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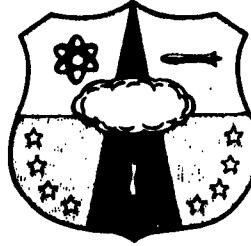
STUDY OF RECOMBINATION PHENOMENA

Volume II. Recombination in Plasma

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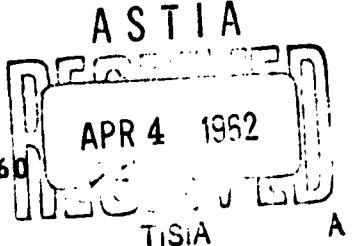
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Research Directorate
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Air Force Systems Command
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New Mexico

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(Prepared under Contract No. AF 29(601)-4143 by H. E. Stubbs,
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Volume II

Recombination in Plasma

FINAL REPORT

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AIR FORCE SPECIAL WEAPONS CENTER
Air Force Systems Command
Kirtland Air Force Base
New Mexico

GEOPHYSICS CORPORATION OF AMERICA
Bedford, Massachusetts

FINAL REPORT

Volume II

Recombination in Plasma

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GCA Technical Report 62-4-A

February 1962

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ABSTRACT

Volume I of this report discusses the radiative and collisional processes which determine the recombination rate in a plasma. A general expression is derived for the recombination rate, and numerical values are given for a hydrogen plasma in the temperature range 250°K to 64,000°K and for all electron densities. These results are applied to an expanding hydrogen plasma and to the expanding debris from a nuclear explosion, and indicate that in an explosion occurring in a vacuum, significant recombination may take place at times later than a millisecond after the detonation.

Volume II contains seven papers dealing with the physics of recombination in plasmas. Included are the radiative transition probabilities for a number of atoms and ions obtained from a theory of atomic screening constants.

PUBLICATION REVIEW

This report has been reviewed and is approved.



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THE STATIONARY PLASMA*

2.1 The Basic Equations

In order to investigate the non-equilibrium properties of a partially ionized plasma, it is necessary to consider the electronic and atomic processes which affect the populations of the individual atomic energy levels. A particular level may be populated by spontaneous and stimulated transitions from other discrete levels, by impact induced transitions from bound states, by radiative recombination of free electrons and by three-body recombination processes involving free electrons. It may be depopulated by the inverse processes of radiative transitions out of the level, impact induced transitions out of the level, photoionization and impact induced ionization.

The increase in population per second of a particular level (p) is given by the differences between the rates of population and depopulation. The equations for the populations in each of the levels will have the form

$$\frac{dn}{dt} = \sum_{j \neq p} a_{jp} n(j) + b_p - a_{pp} n(p) \quad (2-1)$$

In this equation $n(p)$ is the population of the p^{th} level. The expression $a_{jp} n(j)$ appearing in the summation represents the rate at which atoms are entering the p^{th} level from the j^{th} level. The term b_p represents the rate of capture of free electrons into the p^{th} level and the expression $a_{pp} n(p)$ represents the rate at which atoms are

*This chapter is repeated in Volume II to make it available in an unclassified document.

leaving the p^{th} level for other levels and the ionized state. The a's and b's include the effects of both radiative and collision processes, and they are functions of the density and temperature of the free electrons. Explicit expressions for the coefficients are developed in Appendix A.

2.2 Comparison of the Radiative and Collisional Processes

Tables giving the coefficients for the radiative and collisional processes are collected in Appendix A. The tables for hydrogen are essentially complete. For other elements the tables represent a start on the complete assembly of data needed for estimating recombination in complex plasmas. For the present they serve as an indication of the compilation and are useful in showing the pattern of variation of the coefficients.

An examination of the tables shows that the spontaneous transition probabilities decrease rapidly with increasing excitation, in contrast to the collisional excitation and ionization probabilities, which increase rapidly. Thus, from the tables for hydrogen in Appendix A, it may be observed that even if the electron density is as low as 10^{12} cm^{-3} and the electron temperature is as low as 1000°K , electron impact ionization of level $n = 10$ is more rapid than the loss by spontaneous transition. For an electron density of 10^{20} cm^{-3} and an electron temperature of 1000°K , electron impact ionization of the first excited level is more

rapid than the loss by a spontaneous transition. Electronic excitation and de-excitation processes are still more efficient so that a Boltzmann distribution of the highly excited states is to be expected except at low electron densities and temperatures.

2.3 Previous Calculations of Recombination Rates

Baker and Menzel⁽²⁻²⁾ have applied equations of the form of Equation (2-1) to an investigation of the relative intensities of spectral lines in gaseous nebulae in which the ground state of atomic hydrogen is ionized by stellar radiation. In these circumstances, a steady state prevails so that

$$\frac{d}{dt} n(p) = 0$$

and Equation (2-1) reduces to a set of algebraic equations, the solution of which is equivalent to the inversion of a matrix. Baker and Menzel do not distinguish between the individual sub-levels corresponding to a given principal quantum number and consequently assume implicitly that

$$n(n, \ell) = \frac{(2\ell + 1)}{n^2} \sum_{\ell} n(n, \ell) \quad (2-2)$$

Burgess⁽²⁻³⁾ has repeated the calculations taking account of the different sub-levels and he gives the equilibrium populations for electron temperatures of 10,000°K and 20,000°K. He finds that the l -levels are far from being populated according to their statistical weights and that for an optically thin plasma, the p-levels ($l=1$) are much under-populated due to the large probability of np - 1s transitions.

In both investigations, all collision processes are ignored. Although this is a permissible approximation for the low-lying levels of hydrogen when the electron density and the electron temperature are not high (as is the case in most gaseous nebulae), it will ultimately be invalid as n increases.

Since collision processes which redistribute the sub-levels corresponding to a given n , such as

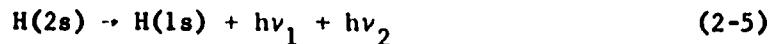


are very efficient, the effect of including collision processes will tend to ensure Equation (2-2). The more refined treatment of Burgess is therefore actually less accurate than that of Baker and Menzel when the electron temperature is high and when the principal quantum number n is large.

Giovanelli⁽²⁻⁴⁾ has included electron collision processes in his treatment, which again assumes statistical equilibrium. In his first paper in which he assumes Equation (2-2), he shows that Saha's ionization

formula applies to the populations of the high-lying levels, provided the electron temperature is employed. This occurs because the most efficient depopulating mechanism is electron impact ionization and the most efficient populating mechanism is the inverse process of three-body recombination and these processes are very rapid. The same situation must apply even in non-equilibrium cases.

In a second paper Giovanelli⁽²⁻⁵⁾ discusses the populations of the low-lying levels. The study contains an inconsistency, which may be serious, in that while he distinguishes between the individual sub-levels, he ignores redistribution processes such as Equation (2-3). His results are therefore invalid at high electron densities and temperatures. We note in passing that his results are also invalid at low electron densities and temperatures in that he ignores the decay of the metastable 2s state by the two-quantum process



Discussions of the hydrogen plasma in non-equilibrium situations have been given by D'Angelo⁽²⁻⁶⁾ and by Bates and Kingston⁽²⁻⁷⁾. In both investigations, heavy particle collisions are ignored and it is assumed that the plasma is optically thin. Both investigations assume Equation (2-2) and ignore processes such as Equation (2-3). This is equivalent to supposing the Equation (2-2) is very fast.

D'Angelo obtains an approximate solution of Equation (2-1) by attempting to follow through in detail the reaction paths of any individual electron, making the assumption that recombination is effective only for

those paths which terminate in the ground state. He ignores the effect of electron impact excitation and de-excitation. He gives results for three electron temperatures, 1000°K , 3000°K and $10,000^{\circ}\text{K}$ and for electron densities in the range from 10^{12} to 10^{13} cm^{-3} only. His investigation reveals the importance of three-body recombination processes (as did the earlier work of Giovanelli) but his method of solution is laborious to apply and the accuracy of the numerical values of the effective recombination coefficients is uncertain.

The method employed by Bates and Kingston is simple and more accurate. They argue that the rates at which atoms in a particular excited state are produced or destroyed are very much greater than the rate at which the very small number density of atoms in that state changes. It follows that for an optically thin plasma except for the ground state

$$\frac{d}{dt} n(p) = 0 \quad (p = 2, 3, \dots) \quad (2-6)$$

so that recombination is effective only into the ground state. Then writing

$$\frac{d}{dt} n(1) = + \alpha_{\text{eff}}(n_e) n_e^2 \quad (2-7)$$

(where $n(1)$ signifies the ground state)

defines the effective recombination coefficient $\alpha_{\text{eff}}(n_e, T_e)$, which will depend upon the electron density as well as the electron temperature.

Their method reduces the set of coupled differential equations, Equation (2-1), to a set of coupled algebraic equations. The number of levels requiring individual examination is restricted since the populations

of the highly excited levels are given by the Saha formula, the level at which this becomes true being provided by the calculations.

2.4 The Number of Discrete Levels

In none of the investigations we have described has the question of the number of levels that should be included in the equations been examined. It is clearly not infinite because ultimately the discrete levels will overlap the continuum.

Ivanov-Kholodnyi, Nikol'skii and Gulyaev⁽²⁻¹⁾ have discussed the lowering of the continuum due to pre-ionization. The treatment is not entirely satisfactory but should suffice for our purposes. They find that the number n_o of levels of different principal quantum number which remain discrete is given by

$$\ln(n_o + 1) = \frac{21.65 - \ln(n_e)}{6} \quad (2-8)$$

Values of n_o have been computed from Equation (2-8) for a wide range of electron densities and they are presented in Figure 2-1. The values are quite large and it seems probable that Stark broadening of the lines will cause a greater effective depression of the levels. The Stark broadening has been discussed by Griem, Kolb and Shen⁽²⁻⁸⁾ and it may be necessary to carry out detailed computations based on their theory. However, the fact that the highly-excited levels are in essentially thermal equilibrium and play only a small role in determining the effective recombination suggests that the solution of the equations is insensitive

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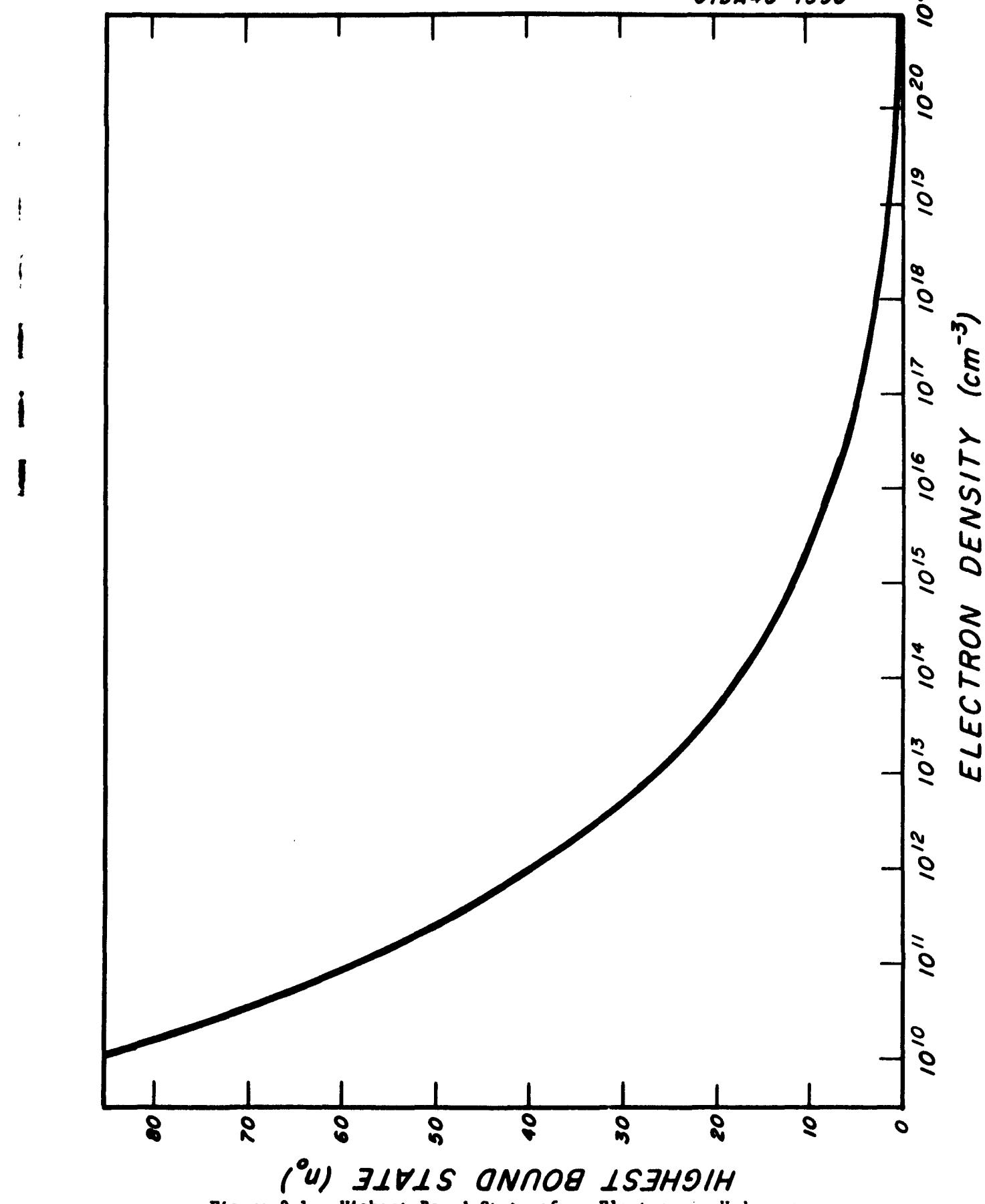


Figure 2-1. Highest Bound State of an Electron in Hydrogen

to the number of levels included. The Stark broadening will be important, however, in determining the opacity, which in turn effects the recombination.

2.5 Computation of Recombination Rate in Optically Thin Hydrogen

Adopting the method of Bates and Kingston⁽²⁻⁷⁾, we first change the variables in Equation (2-1) from $n(p)$ to $\theta(p)$ by introducing the relationship

$$n(p) = n_e n(X^+) \omega_p (h^2/2\pi mkT_e)^{3/2} \exp(-I_p/kT_e) \theta(p) \quad (2-9)$$

(where m is mass of electron, k is Boltzmann's constant, h Planck's constant and I_p the ionization potential of this p^{th} level.)

The new variables $\theta(p)$ are the ratios of populations in the p^{th} levels to the populations derived from the Saha relationship. At equilibrium $\theta(p)$ is unity.

The introduction of (2-9) into Equation (2-1) gives an equation of the form*

$$\frac{d}{dt} \theta(p) = \sum_{j \neq p} a_{jp} n(j) - b_p - a_{pp} \theta(p) \quad p = 1, 2, 3, \dots \quad (2-10)$$

Assuming with Bates and Kingston that

$$\frac{d\theta(p)}{dt} = 0 \quad p = 2, 3, 4, \dots \quad (2-11)$$

*the a's do not have same meanings in Equation (2-10) as in Equation (2-1)

we obtain

$$0 = \sum_{j \neq p} a_{jp} n(j) + b_p - a_{pp} \theta(p) \quad p = 2, 3, 4, \dots \quad (2-12)$$

with the equation for the ground state where $p = 1$ treated as a special case:

$$\frac{d}{dt} \theta(1) = \sum_{j \neq p} a_{j1} \theta(j) + b_1 - a_{11} \theta(1) \quad (2-13)$$

If the series of equations in (2-12) are truncated at some level k , the Equations (2-12) are in the form of $k-1$ linear equations with k unknowns, the unknowns being taken as the θ 's. By inversion of the matrix, a solution may be obtained for all θ 's in terms of one unknown, $\theta(1)$. Because of the linearity of the equations, the solution will have the form

$$\theta(p) = c_0 + c_1 \theta(1) \quad p = 2, 3, \dots, k \quad (2-14)$$

The right side of Equation (2-13) can then be evaluated also in terms of the single unknown $\theta(1)$ and taking account of Equations (2-9) and (2-7), one may obtain the effective recombination coefficient in the form:

$$\alpha_{\text{eff}}(n_e | T_e) = a_0 - a_1 \theta(1) \quad (2-15)$$

Values of a_0 and a_1 in Equation (2-15) have been obtained for an optically thin hydrogen plasma by machine methods for electron temperatures ranging from 250°K to $64,000^{\circ}\text{K}$ and for all electron densities,

TABLE 2-1a
OPTICALLY THIN HYDROGEN ION PLASMA

Quantity a_o appearing in formula (17) for the recombination coefficient α in $\text{cm}^3 \text{sec}^{-1}$.
Except in very hot dense plasmas it suffices to equate α to a_o .

$n(c) \times 10^{-3}$	250	500	1000	2000	4000	8000	16000	32000	64000	α_K
0	4.8^{-12}	3.1^{-12}	2.0^{-12}	1.3^{-12}	7.8^{-13}	4.8^{-13}	2.9^{-13}	1.7^{-13}	1.0^{-13}	1.0^{-13}
10^8	1.4^{-10}	1.8^{-11}	4.7^{-12}	1.9^{-12}	9.5^{-13}	5.2^{-13}	3.0^{-13}	1.8^{-13}	1.0^{-13}	1.0^{-13}
10^9	5.5^{-10}	4.3^{-11}	7.9^{-12}	2.5^{-12}	1.1^{-12}	5.6^{-13}	3.1^{-13}	1.8^{-13}	1.0^{-13}	1.0^{-13}
10^{10}	3.6^{-9}	1.7^{-10}	1.9^{-11}	4.1^{-12}	1.4^{-12}	6.4^{-13}	3.3^{-13}	1.8^{-13}	1.0^{-13}	1.0^{-13}
10^{11}	3.3^{-8}	1.1^{-9}	6.9^{-11}	9.1^{-12}	2.2^{-12}	8.1^{-13}	3.7^{-13}	1.9^{-13}	1.0^{-13}	1.0^{-13}
10^{12}	3.2^{-7}	9.4^{-9}	3.9^{-10}	2.9^{-11}	4.4^{-12}	1.2^{-12}	4.5^{-13}	2.1^{-13}	1.1^{-13}	1.1^{-13}
10^{13}	3.2^{-6}	9.2^{-8}	3.1^{-9}	1.4^{-10}	1.2^{-11}	2.1^{-12}	6.2^{-13}	2.5^{-13}	1.1^{-13}	1.1^{-13}
10^{14}	3.2^{-5}	9.1^{-7}	2.9^{-8}	9.8^{-10}	5.1^{-11}	5.1^{-12}	1.0^{-12}	3.1^{-13}	1.3^{-13}	1.3^{-13}
10^{15}	3.2^{-4}	9.1^{-6}	2.9^{-7}	8.7^{-9}	2.7^{-10}	1.7^{-11}	2.3^{-12}	4.9^{-13}	1.6^{-13}	1.6^{-13}
10^{16}	3.2^{-3}	9.1^{-5}	2.9^{-6}	8.5^{-8}	2.2^{-9}	8.4^{-11}	5.0^{-12}	7.3^{-13}	1.9^{-13}	1.9^{-13}
10^{17}	3.2^{-2}	9.1^{-4}	2.9^{-5}	8.4^{-7}	2.1^{-8}	3.4^{-10}	1.4^{-11}	1.8^{-12}	4.4^{-13}	4.4^{-13}
10^{18}	3.2^{-1}	9.1^{-3}	2.9^{-4}	8.4^{-6}	2.0^{-7}	2.5^{-9}	9.6^{-11}	1.2^{-11}	2.8^{-12}	2.8^{-12}
∞	3.2^{-19}	9.1^{-21}	2.9^{-22}	8.4^{-24}	1.9^{-25}	2.4^{-27}	9.1^{-29}	1.1^{-29}	2.7^{-30}	2.7^{-30}
(cm^{-3})										

The indices give the power of 10 by which the entries must be multiplied.

TABLE 2-1b

Quantity a_1 appearing in formula (17) for the recombination coefficient α in $\text{cm}^3 \text{sec}^{-1}$.

Graph showing $n(c)T^-$ versus ${}^{\circ}\text{K}$ for two values of $n(c)$.

The y-axis is logarithmic, ranging from 10^0 to 10^{18} . The x-axis is linear, ranging from 0 to 64000 K .

Two curves are plotted:

- Solid line:** $n(c) = 9.1$
- Dashed line:** $n(c) = 2.7$

Both curves show a sharp increase in $n(c)T^-$ as temperature decreases below $10,000\text{ K}$.

The indices give the power of 10 by which the entries must be multiplied.

levels up to $n = 10$ being included in the computation. Preliminary values of a_0 and a_1 have been provided by Bates and are given in Tables 2-1a and 2-1b, respectively.

There are certain irregularities in the values as given in the tables which suggest there might be an error in parts of the tabulation. Until a further check of the computations has been completed the values in the table should be regarded as uncertain by a factor of 2.

2.6 Discussion of Computation and Results

In order to illustrate the significance of the differential Equations (2-10), the algebraic Equations (2-12), and the solution as given in Tables 2-1a and 2-1b, it will be worthwhile to consider the changes which take place in the populations of the various excited levels of a hydrogen plasma. Suppose that for an optically thin hydrogen plasma, the temperature and number density of the free electrons are maintained constant by some arbitrary means. Under these conditions, the rate of change of the populations of all the bound states are given by the differential Equations (2-1), and for given initial conditions which assign a value to the population of each of the bound states at the outset, a solution of the Equations (2-1) will give the populations of each of the states for all subsequent time. The general character of this solution is illustrated schematically in Figure 2-2.

In the figure, the populations of the several states are described by the variable θ , which is the ratio of the number in a state to the number in that state under conditions of thermodynamic equilibrium. Since we are supposing that the number density and temperature of the free electrons remains constant,

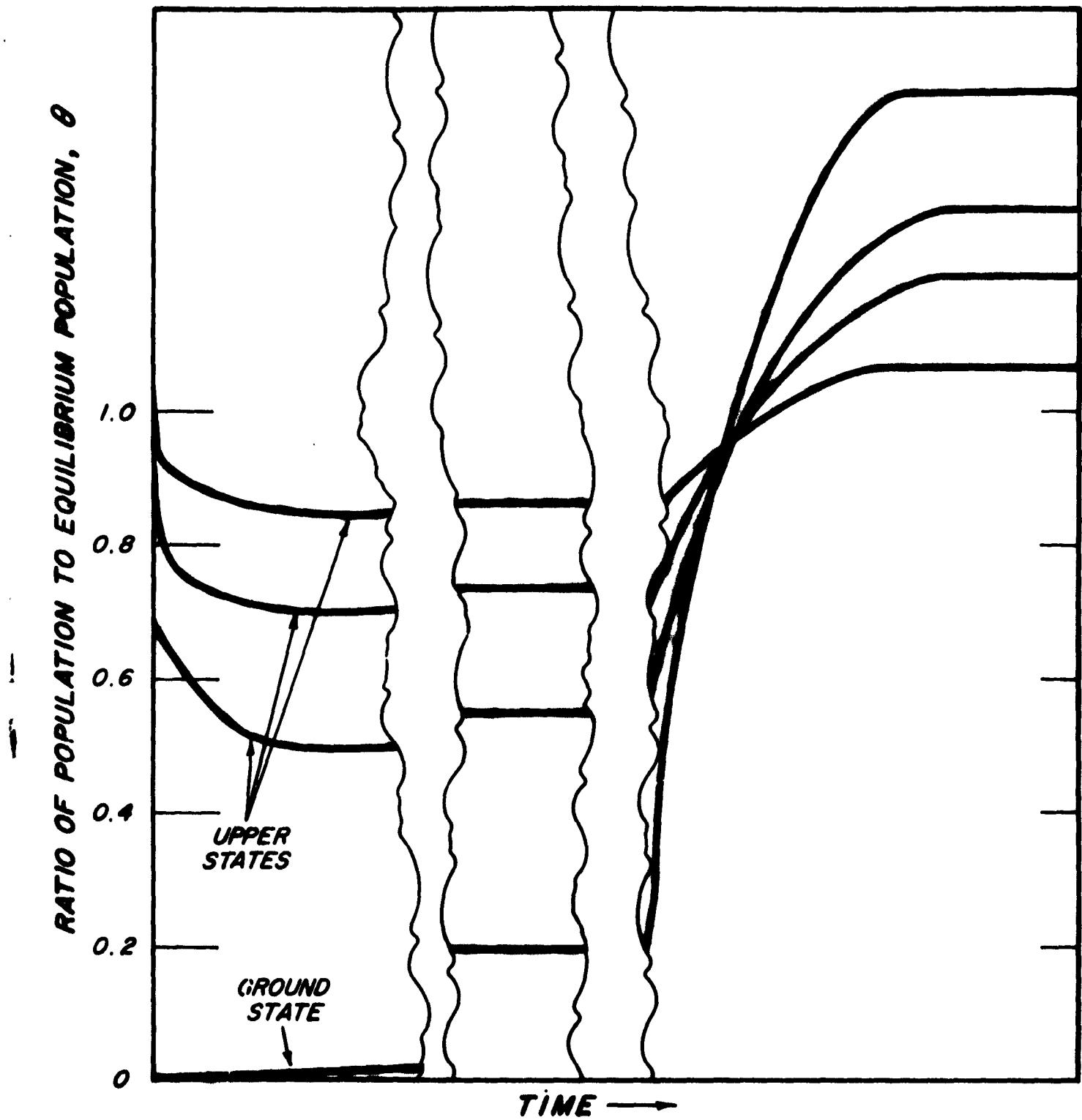


Figure 2-2. Schematic Diagram of Population Changes During Recombination

$\theta(p)$ will be proportional to $n(p)$. In Figure 2-2, it is supposed that the ground state is unpopulated at the outset, but the initial populations of the various excited states are taken at values which have no particular significance. As indicated in the figure, at the outset there will be a very rapid change in the populations of the upper states. In particular, the value of θ for the upper states will change much more rapidly than that of the ground state. After a short time, the rapid changes in θ of the upper states will decline, and a pseudo-steady state will occur such that, if viewed on a short time scale, all the populations remain constant. There will, however, be a non-zero rate of increase in the ground state, which will make itself felt over a longer period of time. This pseudo-steady state condition is represented in Figure 2-2 as occurring just before the first time break, and it is this condition which is described by the algebraic Equations, 2-12 and by their solution obtained taking the recombination coefficient $\alpha = a_0$. At an appreciably later period of time, as represented after the first time break in Figure 2-2, the increase in θ for the ground state will be appreciable, and there will be a corresponding change in the pseudo-steady state values of the populations of the various higher states. This situation is represented in the middle time-period of Figure 2-2, and is also described by the solution to the algebraic Equations, 2-12, but now since $\theta(1)$ is not equal to zero, it is necessary to take the effective recombination rate, as $\alpha = a_0 - a_1\theta(1)$.

The populations of the various states continue to change as recombination proceeds, and the right hand section of Figure 2-2 indicates

the general nature of these changes on a much different time scale than the portions of the figures at the left and the center. The populations will eventually approach asymptotic values at which they are constant, and at which time the net recombination ceases. This condition, which is indicated at the extreme right of the figure represents the steady state under conditions of radiation loss. It can be seen that for this condition, the population of the ground state exceeds that which it would have for thermodynamic equilibrium. The population of the ground state can be obtained readily from the Tables 2-1a and 2-1b by setting $\alpha = a_0 - a_1 \theta(1) = 0$.

In simplifying the differential Equations 2-10, to the corresponding algebraic Equations, 2-12, one gives up any possibility of obtaining information about the initial variation shown at the extreme left of Figure 2-2. Except for this initial response, which is unimportant for the applications considered here, the effective recombination rate and the populations of all the states can be obtained throughout the period illustrated in the second and third time blocks in the Figure from the algebraic equations.

It should be observed that in the procedure followed here, one supposes that the temperature and number density of the free electrons and the conditions on light absorption as described by the χ -parameters are given conditions of the problem. To do otherwise would make the equations (either the differential Equations 2-10 or the algebraic Equations 2-12) non-linear and would vastly increase the difficulties of

obtaining a solution. The solution obtained here can nonetheless be applied to important problems in which the temperature, density and light absorption in the plasma change with time because the pseudo-steady state to which Equation (2-12) applies is achieved in times short compared to those for significant variation in the plasma properties. This matter will be discussed further in Section 3 of Volume I.

2.7 Plasma Other Than Hydrogen

The general plasma has several ionized components each of which can exist in several states of ionization. Nevertheless, the general plasma may be treated in a manner similar to that employed for the hydrogen plasma, but with certain modifications.

Just as for the hydrogen plasma, it is necessary to collect together all the radiative and collisional transition probabilities. Unfortunately, no systematic tabulation of these probabilities has been given even for ground states of systems and the collection of the data is a major task. We have made a beginning in assembling the data and the tabulated value are included in Appendix A.

The basic equations are similar to (2-1) and their solution presents no problem provided heavy particle collisions can be ignored. With this proviso, there is a set of equations of the form (2-1) for each component of the plasma and these sets of equations are uncoupled. The quasi-steady state method may then be applied to each component separately.

It does, in fact, appear reasonable to neglect heavy particle collisions except for charge transfer processes involving the ground states. This exception arises because, although charge transfer into the ground state of a system may be inefficient, it does couple components together and it has a permanent recombining effect. It does not introduce any difficulties into solving the equations since the ground state equation receives special consideration in any event.

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APPENDIX A
A. Dalgarno, A. Naqvi, E. Ashley and H. E. Stubbs

ATOMIC PROCESSES IN A RECOMBINING PLASMA

The time dependence of the population of each state of a recombining plasma can be obtained from a consideration of the several processes by which the atoms enter and leave a given state. Both radiative and collisional processes must be considered.

A.1 Radiative Transitions Between Bound States

The rate of depopulation of the state p by spontaneous transitions to lower states q , may be written

$$n(p) \sum_{q < p} A(p, q) \quad (A-1)$$

where $A(p, q)$ is the probability of a spontaneous transition from the state p to the state q measured in sec^{-1} .

If the plasma is not optically thin, stimulated emissions and absorptions occur. For the rate of upward transitions which depopulate the state p , we write

$$\frac{n(p)}{\omega_p} \sum_{r > p} \omega_r \chi(p, r) A(r, p) \quad (A-2)$$

where ω_p is the statistical weight of the state p and $\chi(p, r)$ is a factor which takes account of the opacity. In particular for a plasma in thermodynamic equilibrium with the radiation field

$$\chi(r,p) = \left\{ \exp \left(\frac{h\nu_{rp}}{kT} \right) \right\}^{-1} \quad (A-3)$$

where ν_{rp} is the energy of the $r - p$ transition. For an optically thin plasma, χ vanishes. The rate of stimulated downward transitions can be written

$$n(p) \sum_{q>p} \chi(p,q) A(p,q) \quad (A-4)$$

The p state can also be populated by bound-bound radiative transitions and we have for the rates of population by the three processes

$$\sum_{r>p} n(r) A(r,p) \quad (A-5)$$

$$\sum_{r>p} n(r) \chi(r,p) A(r,p) \quad (A-6)$$

$$\omega_p \sum_{q<p} \frac{n(q)}{\omega_q} \chi(q,p) A(p,q) \quad (A-7)$$

The probability of a spontaneous transition from a level p to a lower level q may be expressed in the form

$$A(p,q) = \frac{64\pi \nu^3}{3hc \omega_p} S(p,q) \quad (A-8)$$

where ν is the frequency of the emitted radiation, ω_p is the statistical weight of the p^{th} level and $S(p,q)$ is the transition strength, defined according to

$$S(p,q) = e^2 \left| \langle \Psi_p, \sum_j \vec{r}_j \Psi_q \rangle \right| \quad (A-9)$$

where Ψ_p and Ψ_q are the configurations of the initial and final states and \vec{r} is the position vector of the j^{th} electron. In the case of Russell-Saunders coupling, $S(p,q)$ reduces to the form

$$S(p,q) = \mathcal{F}(L) \mathcal{F}(M) \sigma^2 \quad (\text{A-10})$$

where $\mathcal{F}(L)$ is the relative strength of a multiplet within a transition array, $\mathcal{F}(M)$ is the relative strength of a line within a multiplet and σ is a transition integral involving radial wave functions only. Tables of $\mathcal{F}(L)$ and $\mathcal{F}(M)$ are available for most multiplets (Goldberg^(A-1), White and Eliason^(A-2), Russell^(A-3), Allen^(A-4), and if necessary, they can easily be extended following Rohrlich^(A-5)). The transition integral σ presents greater difficulties. If $R(n\ell|r)$ is the initial radial wave function of the active electron and $R(n'\ell'|r)$ is the final wave function,

$$\sigma^2 = \frac{1}{4\pi^2 \cdot 1} \left\{ \int_0^\infty R(n\ell|r) r^3 R(n'\ell'|r) dr \right\}^2 \quad (\text{A-11})$$

where ℓ is the lower of the azimuthal quantum numbers ℓ and ℓ' which characterize the active electrons.

For hydrogen, values of $\sigma^2(n\ell, n'\ell')$ have been computed by Green, Rush and Chandler^(A-6) and the corresponding values of $A(n\ell, n'\ell')$ for n and n' less than or equal to 8 are presented in Table A-1. Of interest also are the total transition probabilities $A(n, n')$ obtained by summing $A(n\ell, n'\ell')$ over all possible values of ℓ and ℓ' consistent with n and n' , assuming that the sub-levels are distributed according to their statistical weights. The total transition probabilities so obtained are

TABLE A-1
TRANSITION PROBABILITIES FOR HYDROGEN IN sec⁻¹
 $A(nL, n'L')$

Trans ition n n	2	3	4	5	6	7	8
np - 1s	6.258(8)	1.671(8)	6.811(7)	3.434(7)	1.971(7)	1.235(7)	8.246(6)
np - 2s		2.244(7)	9.665(6)	4.947(6)	2.858(6)	1.797(6)	1.202(6)
ns - 2p		6.312(6)	2.577(6)	1.288(6)	7.348(5)	4.585(5)	3.053(5)
nd - 2p		6.463(7)	2.062(7)	9.423(6)	5.144(6)	3.130(6)	2.052(6)
np - 3s			3.064(6)	1.637(6)	9.549(5)	6.024(5)	4.033(5)
ns - 3p			1.835(6)	9.045(5)	5.070(5)	3.127(5)	2.065(5)
nd - 3p			7.036(6)	3.391(6)	1.877(6)	1.149(6)	7.551(5)
np - 3d			3.475(5)	1.495(5)	7.822(4)	4.635(4)	2.983(4)
nf - 3d			1.378(7)	4.541(6)	2.145(6)	1.207(6)	7.531(5)
np - 4s				7.370(5)	4.455(5)	2.827(5)	1.895(5)
ns - 4p				6.449(5)	3.581(5)	2.173(5)	1.418(5)
nd - 4p				1.485(6)	8.619(5)	5.336(5)	3.520(5)
np - 4d				1.884(5)	9.414(4)	5.389(4)	3.392(4)
nf - 4d				2.584(6)	1.287(6)	7.337(5)	4.605(5)
nd - 4f				5.045(4)	2.144(4)	1.123(4)	6.697(3)
ng - 4f				4.253(6)	1.372(6)	6.456(5)	3.639(5)
np - 5s					2.427(5)	1.589(5)	1.070(5)
ns - 5p					2.679(5)	1.616(5)	1.039(5)
nd - 5p					4.490(5)	2.899(5)	1.931(5)

TABLE A-1 (continued)

Trans ition	2	3	4	5	6	7	8
np - 5d				9.583 (4)	5.302 (4)	3.242 (4)	
nf - 5d				7.225 (5)	4.326 (5)	2.751 (5)	
nd - 5f				3.903 (4)	1.909 (4)	1.087 (4)	
ng - 5f				1.104 (6)	5.476 (5)	3.131 (5)	
nf - 5g				1.136 (4)	4.647 (3)	2.386 (3)	
nh - 5g				1.643 (6)	5.082 (5)	2.336 (5)	
np - 6s					9.779 (4)	6.772 (4)	
ns - 6p					1.264 (5)	8.096 (4)	
nd - 6p					1.702 (5)	1.178 (5)	
np - 6d					5.099 (4)	3.037 (4)	
nf - 6d					2.591 (5)	1.724 (5)	
nd - 6f					2.521 (4)	1.360 (4)	
ng - 6f					3.760 (5)	2.260 (5)	
nf - 6g					1.109 (4)	5.231 (3)	
nh - 6g					5.317 (5)	2.575 (5)	
ng - 6h					3.351 (3)	1.304 (3)	
n1 - 6h					7.400 (5)	2.173 (5)	
np - 7s						4.529 (4)	
ns - 7p						6.562 (4)	
nd - 7p						7.533 (4)	

TABLE A-1 (continued)

Trans- ition	1	2	3	4	5	6	7	8
np - 7d								2.870(4)
nf - 7d								1.100(5)
nd - 7f								1.591(4)
ng - 7f								1.534(5)
nf - 7g								8.459(3)
nh - 7g								2.089(5)
ng - 7h								3.851(3)
ni - 7h								2.803(5)
nh - 7i								1.189(3)
nk - 7i								3.721(5)

presented in Table A-2. There are occasional differences from previous tabulations of Menzel and Pekeris^(A-7).

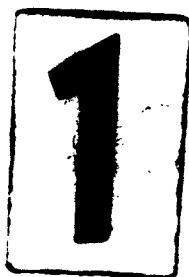
For more complex systems, approximations must be made. For many cases and especially for the excited states of light elements, the Coulomb approximation of Bates and Damgaard^(A-8) should be adequate. In this approximation the active electron is regarded as moving in the field of an effective nuclear charge being determined from the observed ionization potentials for the states. Bates and Damgaard have presented tables from which σ^2 may be determined for transitions involving small values of ℓ and ℓ' and we have used them to calculate the transition probabilities of the more important lines of Li I, Li II, C I, C II, C III, N I, N II, N III, O I, O II and O III. The results, illustrative of the information which may be obtained by the Bates and Damgaard methods, are presented in Table A-3. Also, Table A-4 lists the results of calculations by this method of the transition probabilities of resonance lines of a number of atoms of interest.

For heavier elements it may not be possible to apply the Coulomb approximation since the ionization potentials are not always known and a less empirical approximation scheme is required. A theory using screening constants, which is described in the following appendices, is capable of dealing with these cases.

TABLE A-2
 TOTAL TRANSITION PROBABILITIES FOR HYDROGEN IN sec^{-1}
 $A(n, n')$

n'	1	2	3	4	5	6	7	8	9	10	11
n											
1	-	-	-	-	-	-	-	-	-	-	-
2	4.696 (8)	-	-	-	-	-	-	-	-	-	-
3	5.572 (7)	4.410 (7)	-	-	-	-	-	-	-	-	-
4	1.278 (7)	8.419 (6)	8.986 (6)	-	-	-	-	-	-	-	-
5	4.122 (6)	2.530 (6)	2.201 (6)	2.699 (6)	-	-	-	-	-	-	-
6	1.643 (6)	9.732 (5)	7.783 (5)	7.710 (5)	1.025 (6)	-	-	-	-	-	-
7	7.564 (5)	4.389 (5)	3.358 (5)	3.041 (5)	3.251 (5)	4.558 (5)	-	-	-	-	-
8	3.867 (5)	2.215 (5)	1.650 (5)	1.423 (5)	1.381 (5)	1.560 (5)	2.271 (5)	-	-	-	-
9	2.141 (5)	1.216 (5)	8.904 (4)	7.455 (4)	6.904 (4)	7.061 (4)	8.232 (4)	1.232 (5)	-	-	-
10	1.262 (5)	7.122 (4)	5.156 (4)	4.232 (4)	3.798 (4)	3.686 (4)	3.903 (4)	4.674 (4)	7.147 (4)	-	-
11	7.829 (4)	4.397 (4)	3.156 (4)	2.555 (4)	2.245 (4)	2.108 (4)	2.116 (4)	2.299 (4)	2.811 (4)	4.374 (4)	-
12	5.063 (4)	2.834 (4)	2.021 (4)	1.620 (4)	1.402 (4)	1.288 (4)	1.250 (4)	1.286 (4)	1.426 (4)	1.773 (4)	2.797 (
13	3.391 (4)	1.893 (4)	1.343 (4)	1.068 (4)	9.143 (3)	8.267 (3)	7.841 (3)	7.799 (3)	8.187 (3)	9.226 (3)	1.163 (
14	2.340 (4)	1.303 (4)	9.211 (3)	7.284 (3)	6.181 (3)	5.523 (3)	5.153 (3)	5.007 (3)	5.007 (3)	5.414 (3)	6.182 (
15	1.656 (4)	9.210 (3)	6.490 (3)	5.108 (3)	4.306 (3)	3.813 (3)	3.514 (3)	3.357 (3)	3.323 (3)	3.422 (3)	3.876 (
16	1.199 (4)	6.658 (3)	4.680 (3)	3.669 (3)	3.007 (3)	2.705 (3)	2.469 (3)	2.329 (3)	2.267 (3)	2.278 (3)	2.376 (
17	8.852 (3)	4.910 (3)	3.444 (3)	2.692 (3)	2.248 (3)	1.965 (3)	1.780 (3)	1.663 (3)	1.597 (3)	1.577 (3)	1.605 (
18	6.650 (3)	3.685 (3)	2.580 (3)	2.012 (3)	1.674 (3)	1.456 (3)	1.311 (3)	1.215 (3)	1.156 (3)	1.126 (3)	1.126 (
19	5.074 (3)	2.809 (3)	1.964 (3)	1.528 (3)	1.268 (3)	1.099 (3)	9.844 (2)	9.065 (2)	8.550 (2)	8.248 (2)	8.136 (
20	3.925 (3)	2.172 (3)	1.517 (3)	1.178 (3)	9.746 (2)	8.419 (2)	7.512 (2)	6.882 (2)	6.449 (2)	6.170 (2)	6.023 (

The brackets give the powers of 10 by which the entries must be multiplied.



DROGEN IN sec⁻¹

	8	9	10	11	12	13	14	15	16	17	18	19
-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-
i)	-	-	-	-	-	-	-	-	-	-	-	-
i)	1.232 (5)	-	-	-	-	-	-	-	-	-	-	-
i)	4.674 (4)	7.147 (4)	-	-	-	-	-	-	-	-	-	-
i)	2.299 (4)	2.811 (4)	4.374 (4)	-	-	-	-	-	-	-	-	-
i)	1.286 (4)	1.426 (4)	1.773 (4)	2.797 (4)	-	-	-	-	-	-	-	-
i)	7.799 (3)	8.187 (3)	9.226 (3)	1.163 (4)	1.856 (4)	-	-	-	-	-	-	-
i)	5.007 (3)	5.007 (3)	5.414 (3)	6.182 (3)	7.880 (3)	1.270 (4)	-	-	-	-	-	-
i)	3.357 (3)	3.323 (3)	3.422 (3)	3.876 (3)	4.268 (3)	5.493 (3)	8.928 (3)	-	-	-	-	-
i)	2.329 (3)	2.267 (3)	2.278 (3)	2.376 (3)	2.595 (3)	3.024 (3)	3.923 (3)	6.425 (3)	-	-	-	-
i)	1.663 (3)	1.597 (3)	1.577 (3)	1.605 (3)	1.692 (3)	1.865 (3)	2.191 (3)	2.863 (3)	4.717 (3)	-	-	-
i)	1.215 (3)	1.156 (3)	1.126 (3)	1.126 (3)	1.158 (3)	1.232 (3)	1.368 (3)	1.619 (3)	2.128 (3)	3.528 (3)	-	-
i)	9.065 (2)	8.550 (2)	8.248 (2)	8.136 (2)	8.219 (2)	8.527 (2)	9.139 (2)	1.022 (3)	1.217 (3)	1.609 (3)	2.679 (3)	-
i)	6.882 (2)	6.449 (2)	6.170 (2)	6.023 (2)	6.002 (2)	6.116 (2)	6.394 (2)	6.899 (2)	7.763 (2)	9.291 (2)	1.234 (3)	2.066 (3)

TABLE A-3

BOUND-BOUND TRANSITION PROBABILITIES A(p,q) FOR THE IMPORTANT LINES OF LiI, LiIII, CI, CII, CIII, NI, NII, NIII, OI, OII AND OIII

LiI Lines

Transition	J ₂	J ₁	λ(Å)	σ ²	A(10 ⁷ sec ⁻¹)
2p ² P ⁰ -2s ² S	1/2	1/2	6709.8	5.424	3.63
	3/2	1/2	6709.6	5.424	3.63
3p ² P ⁰ -2s ² S	1/2	1/2	3233.6	0.01641	0.098*
	3/2	1/2	3233.6	0.01641	0.098*
4p ² P ⁰ -2s ² S	1/2	1/2	2742.0	0.01392	0.136*
	3/2	1/2	2742.0	0.01392	0.136*
5p ² P ⁰ -2s ² S	1/2	1/2	2563.0	3.90x10 ⁻³	0.0468*
	3/2	3/2	2563.0	3.90x10 ⁻³	0.0468*

LiIII Lines

Transition	λ(Å)	f _(m)	σ ²	A(10 ⁷ sec ⁻¹)
1s2p ¹ P ⁰ -1s ² 1S	199.3	6	3.72x10 ⁻⁵	1.90*
1s3p ¹ P ⁰ -1s ² 1S	178.0	6	9.647x10 ⁻³	691
1s4p ¹ P ⁰ -1s ² 1S	171.6	6	3.219x10 ⁻³	257

CI Lines

2p(² P ⁰)3s ³ P ⁰ -2p ² ³ P	1657	18	0.01397	1.24*
2s2p ³ ³ D ⁰ -2s ² 2p ² ³ P	1561	30	00.9563	101
2s2p ³ ³ P ⁰ -2s ² 2p ² ³ P	1329	18	0.01284	2.21*
2p(² P ⁰)4s ³ P ⁰ 2p ² ³ P	1280	18	0.001488	0.287*

*below 90% maximum value

TABLE A-3 (continued)

CII Lines

Transition	$\lambda(\text{\AA})$	$\mathcal{S}(\text{M})$	σ^2	$A(10^7 \text{ sec}^{-1})$
$2s2p^2 2D-2s^2 2p^2 P^o$	1335		1.096	
$2s2p^2 2S-2s^2 2p^2 P^o$	1037		1.047	
$2s2p^2 2P-2s^2 2p^2 P^o$	904		0.8418	
$2s^2 3s^2 S-2s^2 2p^2 P^o$	858	6	0.062	59.4*
$2s^2 (1S)3d^2 D-2s^2 2p^2 P^o$	687	60	0.04008	1500
$2s^2 (1S)4s^2 S-2s^2 2p^2 P^o$	636	6	0.00817	20.8*
$2s^2 (1S)4d^2 D2s^2 2p^2 P^o$	595	60	0.01357	78.0*
$2s^2 (1S)5s^2 S2s^2 2p^2 P^o$	577	6	0.002743	8.64*
$2s^2 (1S)Sd^2 D-2s^2 2p^2 P^o$	560	60	0.005464	37.7*

CIII Lines

$2s(^2S)2p^1 P^o-2s^2 1S$	977	6	0.5723	248
$2s(^2S)3p^1 P^o-2s^2 1S$	386	6	0.05579	392
$2s(^2S)4p^1 P^o-2s^2 1S$	310	6	0.006529	88.5

NI Lines

$2s^2 2p^2 (^3P)3s^4 P^-$				
$2s^2 2p^3 4S^o$	1200	12	0.007382	0.860*
$2p^2 (^3P)4s^4 P-2p^3 4S^o$	964	12	0.0007751	0.175*
$2p^2 (^3P)3d^4 P-2p^3 4S^o$	953	120	0.04008	93.7
$2s2p^4 4P-2s^2 2p^3 4S^o$	1135	1135	0.5631	
$2p^2 (^3P)5s^4 P-2p^3 4S^o$	911	12	0.0003190	0.0853*

*Below 90% maximum value

TABLE A-3 (continued)

NII Lines

Transition	$\lambda(\text{\AA})$	$\mathcal{L}(\text{M})$	σ^2	$A(10^7 \text{ sec}^{-1})$
$2s2p^3 3D^0 - 2s^2 sp^2 3P$	1085	30	0.3732	148
$2s2p^3 3P^0 - 2s^2 2p^2 3P$	916	18	0.3884	195
$2p(^2P^0)3s^3P^0 - 2p^2 3P$	671	18	0.01671	22.3
$2s2p^3 3S^0 - 2s^2 2p^2 3P$	645	12	0.01833	55.2
$2p(^2P^0)3d^3D^0 - 2p^2 3P$	534	135	0.00729	109

NIII Lines (C.A.)

$2s2p^2 2D - 2s^2 2p^2 P^0$	991		0.1947	
$2s2p^2 2S - 2s^2 2p^2 P^0$	764		0.2135	
$2s2p^2 2P - 2s^2 2p^2 P^0$	686		0.1986	
$2s^2 (^1S)3s^2 S - 2s^2 2p^2 P^0$	452	6	0.01173	77.1
$2s^2 (^1S)3d^2 D - 2s^2 2p^2 P^0$	374	60	0.01028	238
$2s^2 (^1S)4s^2 S - 2s^2 2p^2 P^0$	332	6	0.001995	33.0
$2s2p(^3P^0)3p^2 P - 2s^2 2p^2 P^0$	324		0.006543	
$2s^2 (^1S)4d^2 D - 2s^2 2p^2 P^0$	309	60	0.00149	61.2

OI Lines

$2p^3 (^4S^0)3s^3S^0 - 2p^4 3P$	1303	12	0.01261	4.62
$2p^3 (^4S^0)4s^3S^0 - 2p^4 3P$	1040	12	0.001584	1.14
$2p^3 (^4S^0)3d^3D^0 - 2p^4 3P$	1027		0.03764	
$2p^3 (^2D^0)3s^3D^0 - 2p^4 3P$	989	15	0.0007629	0.160*
$2p^3 (^4S^0)2s^3S^0 - 2p^4 3P$	977	12	0.004858	4.20

*Below 90% maximum value

TABLE A-3 (continued)

OII Lines (C.A.)

Transition	$\lambda(\text{\AA})$	$\mathcal{L}(\text{M})$	σ^2	$A(10^7 \text{ sec}^{-1})$
$2s2p^4 4P - 2s^2 2p^3 4S^o$	834		0.2670	
$2s^2 2p^2 (3P) 3s^4P -$				
$2s^2 2p^3 4S^o$	539	12	0.006351	8.2*
$2p^2 (3P) 3d^4P - 2p^3 4S^o$	430	120	0.005050	128
$2p^2 (3P) 3d^4D - 2p^3 4S^o$	430		0.005356	

OIII Lines

$2s2p^3 3D^o - 2s^2 2p^2 3P$	834	30	0.1417	98.4*
$2s2p^3 3P^o - 2s^2 2p^2 3P$	703	18	0.1538	179
$2s2p^3 3S^o - 2s^2 2p^2 3P$	508	12	0.1643	1014
$2s^2 2p^2 (2P^o) 3s^3P^o -$				
$2s^2 2p^2 3P$	374	18	0.006293	48.6*
$2s^2 2p^2 (2P^o) 3d^3D^o -$				
$2s^2 2p^2 3P$	306	135	0.005453	346

*Below 90% maximum value

TABLE A-4
TRANSITION PROBABILITIES FOR RESONANCE LINES

Element	Transition (Upper - Lower)	$J_2 - J_1$	$\lambda(\text{\AA})$	σ^2	$A(10^6 \text{ sec}^{-1})$
Rb I	$4p^6(^1S)5p \ 2p^0 -$ $4p^6(^1S)5s \ 2s$	$1/2 - 1/2$	7947.60	8.82	35.5
Sr I	$5s(^2S)5p \ 1p^0 -$ $5s^2 \ 1s$	$1 - 0$	4607.331	4.72	195
Sr II	$4p^6(^1S)5p \ 2p^0 -$ $4p^6(^1S)5s \ 2s$	$1 \ 1/2 - 1/2$	4077.714	4.92	147
Zr I	$4d^2 5s(^4F)5p \ 3F^0 -$ $4d^2 5s^2 \ 3F$	$4 - 4$ $2 - 2$	6121.49 6134.58	3.19	52.5 49.6
Zr II	$4d^2(^3F)5p \ 4G^0 -$ $4d^2(^3F)5s \ 4F$	$5 \ 1/2 - 4 \ 1/2$	3391.96	3.59	186
Nb I	$4d^3 5s(^5F)5p \ 6F^0 -$ $4d^4(^5D)5s \ 6D$	$5 \ 1/2-4 \ 1/2$	4058.933	3.39	410
Mo I	$4d^5(^6S)5p \ 7p^0 -$ $4d^5(^6S)5s \ 7s$	$4 - 3$ $3 - 3$ $2 - 3$	3798.359 3864.115 3902.968	3.35	123 117 114
Tc I	$5d^5 5s(^7S)5p \ 6p^0 -$ $5d^5 5s^2 \ 6s$	$3 \ 1/2-2 \ 1/2$ $2 \ 1/2-2 \ 1/2$ $1 \ 1/2-2 \ 1/2$	4298.2 4263.4 4239.4	3.15	160 164 167
Ru I	$4d^7(^4F)5p \ 5D^0 -$ $4d^7(^4F)5s \ 5P$	Entire Multiplet	3799.124	3.27	120

TABLE A-4 (continued)

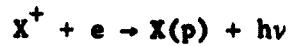
Element	Transition (Upper - Lower)	$J_2 - J_1$	$\lambda(\text{\AA})$	σ^2	$A(10^6 \text{ sec}^{-1})$
Rh I	$4d^8(^3F)5p\ 4D^0 -$	$3\ 1/2-4\ 1/2$	3692.357	3.21	115
	$4d^8(^3F)5s\ 4F$	$2\ 1/2-3\ 1/2$	3657.987		1082
Ag I	$4d^{10}(^1S)5p\ 2P^0 -$	$1\ 1/2-1/2$	3280.682	2.95	169
	$4d^{10}(^1S)5s\ 2S$	$1/2-1/2$	3382.890		154
Cd I	$4d^{10}5s0(^2S)5p\ 1P^0 -$	$1-0$	2288.7	1.99	671
	$4d^{10}5s2(^1S)$				
In I	$5s^2(^1S)6s\ 2S -$	$1/2-1\ 1/2$	4511.310	0.890	39.2
	$5s^2(^1S)5p\ 2P^0$	$1/2-1/2$	4101.764		26.1
Sn I	$5s^25p(^2P_1)6s\ 3P^0 -$	$1-2$	3175.046	0.202	10.6
	$5s^25p^2\ 3P^2$	$0-1$	3034.120		29.2
Cs I	$5p^6(^1S)6p\ 2P^0 -$	$1\ 1/2-1/2$	8521.10	9.94	32.5
	$5p^6(^1S)6s\ 2S$	$1/2-1/2$	8943.50		28.1
Ba I	$6s(^2S)6p\ 1P^0 -$	$1-0$	5535.484	5.78	138
	$6s^2(^1S)$				
Ba II	$5p^6(^1S)6p\ 2P^0 -$	$1\ 1/2-1/2$	4554.033	5.96	127
	$5p^6(^1S)6s\ 2S$	$1/2-1/2$	4934.086		100
La I	$5d6s(^1D)6p\ 2D^0 -$	$2\ 1/2-2\ 1/2$	7270.11	5.10	50.0
	$5d6s^2\ 2D$				

TABLE A-4 (continued)

Element	Transition (Upper - Lower)	$J_2 - J_1$	$\lambda(\text{\AA})$	σ^2	$A(10^6 \text{ sec}^{-1})$
Rh I	$4d^8(^3P)5p\ 4D^0 -$	3 1/2-4 1/2	3692.357	3.21	115
	$4d^8(^3P)5s\ 4F$	2 1/2-3 1/2	3657.987		1082
Ag I	$4d^{10}(^1S)5p\ 2P^0 -$	1 1/2- 1/2	3280.682	2.95	169
	$4d^{10}(^1S)5s\ 2S$	1/2 - 1/2	3382.890		154
Cd I	$4d^{10}5s0(^2S)5p\ 1P^0 -$	1 - 0	2288.7	1.99	671
	$4d^{10}5s^2\ 1S$				
In I	$5s^2(^1S)6s\ 2S -$	1/2- 1 1/2	4511.310	0.890	39.2
	$5s^2(^1S)5p\ 2P^0$	1/2 - 1/2	4101.764		26.1
Sn I	$5s^25p(^2P^0_1)6s\ 3P^0 -$	1 - 2	3175.046	0.202	10.6
	$5s^25p^2\ 3P^2$	0 - 1	3034.120		29.2
Cs I	$5p^6(^1S)6p\ 2P^0 -$	1 1/2- 1/2	8521.10	9.94	32.5
	$5p^6(^1S)6s\ 2S$	1/2 - 1/2	8943.50		28.1
Ba I	$6s(^2S)6p\ 1P^0 -$	1 - 0	5535.484	5.78	138
	$6s^2\ 1S$				
Ba II	$5p^6(^1S)6p\ 2P^0 -$	1 1/2- 1/2	4554.033	5.96	127
	$5p^6(^1S)6s\ 2S$	1/2 - 1/2	4934.086		100
La I	$5d6s(^1D)6p\ 2D^0 -$	2 1/2-2 1/2	7270.11	5.10	50.0
	$5d6s^2\ 2D$				

A.2 Radiative Bound-Free Transitions

In order to calculate the coefficient $\alpha(p)$ for radiative capture of electrons into state p



we must make some assumption about the electron velocity distribution.

Since the electrons exchange energy readily in elastic collisions, they may be described by a Maxwellian distribution characterized by an electron temperature T_e . The recombination coefficient is accordingly

$$\alpha(p|T_e) = \frac{1}{c^2} \left(\frac{2}{\pi} \right)^{1/2} \left(\frac{mkT_e}{2\omega_p} \right)^{-3/2} \exp(-I_p/kT_e) \times \int_{I_p}^{\infty} Q_\nu(p) (h\nu)^2 \exp(-h\nu/kT_e) [1 + X(\nu)] d(h\nu) \quad (A-12)$$

where I_p is the ionization potential of the p^{th} level, $h\nu$ is energy of the radiation photon and $Q_\nu(p)$ is the photoionization cross section corresponding to the process



The rate of population by radiative capture is

$$\alpha(p|T_e) n_e n(X^+) \quad (A-14)$$

where n_e and $n(X^+)$ are respectively the electron and X^+ ion number densities.

The rate of depopulation by photoionization may be written

$$n(p) \beta(p)$$

where

$$\beta(p) = \frac{8\pi}{h^2 c^2} \int_{I_p}^{\infty} Q_{\nu}(p) h\nu (h\nu) d(h\nu) \quad (A-15)$$

The quantal description of bound-free transitions is entirely similar to that of bound-bound transitions except that the radial wave function $R(n'l'|r)$ in (A-11) becomes $R(\epsilon'l'|r)$, describing an electron of positive energy ϵ' moving in the field of the ion. Thus, the cross section for the transition of an electron from the bound state (nl) to the continuum state of energy ϵ' is

$$Q_{\nu}(nl; \epsilon') = \frac{4\pi\alpha_0^2}{3} \left(\frac{I_n + \epsilon'}{2} \right) \sum_{l'=\pm 1} |C_{l'}| |g(nl; \epsilon'l')|^2 \quad (A-16)$$

where I_n is the ionization potential, $C_{l'}$ are simple algebraic quantities which depend upon the initial and final atomic configurations and $g(nl; \epsilon'l')$ is a radial transition integral

$$g(nl; \epsilon'l') = I_{nl} \int_0^{\infty} r^3 R(nl|r) R(\epsilon'l'|r) dr \quad (A-17)$$

Although exact analytical expressions are available for the matrix elements describing the photoionization of the excited states of hydrogen (Gordon ^(A-9)), they are complicated and have not yet been given a numerical form except for the lowest lying levels. Giovanelli ^(A-10) employs an approximate formula due to Gaunt ^(A-11) for the photoionization cross section of level p at a frequency ν

$$Q_{\nu}(p) = \frac{64\pi^4}{3\sqrt{3}} \frac{me^{10}}{c h^6} \frac{1}{p^{5/3}} \quad (A-18)$$

which in numerical form is

$$Q_v(p) = \frac{2.82 \times 10^{29}}{p^5 v^3} \text{ (cm}^2\text{)} \quad (\text{A-19})$$

This choice has also been made by Elwert^(A-12) and Ivanov-Kholodnyi et al.,^(A-13) but it is of questionable accuracy. Recently, Burgess^(A-14) has presented tables useful for low velocities of the ejected electron, from which more accurate photoionization cross sections may be obtained for a hydrogen plasma. His calculations distinguish between the various sub-levels and apply to all levels with $p \leq 12$.

Using his calculations, the radiative recombination coefficients may be calculated according to (A-12) and Burgess has given values of $\alpha(n\ell|T_e)$ for electron temperatures of $10,000^{\circ}\text{K}$ and $20,000^{\circ}\text{K}$. We do not wish to distinguish between the individual sub-levels (except possibly in the latest stages of the plasma decay). For a hydrogenic plasma of nuclear charge Z , after suitably averaging over the sub-levels, we obtain the formula (Seaton^(A-15)):

$$\alpha(p, Z|T_e) = DZ x_p^{3/2} s_p(\lambda) \quad (\text{A-20})$$

where

$$D = \frac{2^6}{3} \left(\frac{\pi}{3} \right)^{\frac{1}{2}} \alpha_f^4 c a_0^2 = 5.197 \times 10^{-14} \text{ cm}^3 \text{ sec}^{-1} \quad (\text{A-21})$$

$$\lambda = \frac{hRcZ^2}{kT_e} = \frac{157890Z^2}{T_e} \quad (\text{A-22})$$

and

$$s_p(\lambda) = s^{(0)}(x_p) + \lambda^{-1/3} s^{(1)}(x_p) + \lambda^{-2/3} s^{(2)}(x_p) \quad (\text{A-23})$$

with

$$s^{(0)}(x) = \exp(-x) Ei(x) \quad (A-24)$$

$$s^{(1)}(x) = 0.1728 x^{1/3} \int_0^{\infty} (u+1)^{-5/3} (u-1) e^{-xu} du \quad (A-25)$$

$$s^{(2)}(x) = -0.0496 x^{2/3} \int_0^{\infty} (u+1)^{-7/3} (u^2 + \frac{4}{3}u + 1) e^{-xu} du \quad (A-26)$$

$$x_n = \frac{\lambda}{p^2} \cdot \frac{1}{kT_e} \cdot \frac{15.788}{p^2} z^2, \quad Ei(x) = \int_x^{\infty} \frac{e^{-v}}{v} dv \quad (A-27)$$

Seaton (A-15) has published tables of $xs^{(0)}(x)$, $xs^{(1)}(x)$ and $xs^{(2)}(x)$, from which the radiative recombination coefficients $\alpha(p, Z|T_e)$ may be calculated readily. Values obtained for hydrogen ($Z=1$) in this way have been provided by Bates and are shown in Table A-5. Seaton also presents tables similar to those for the $xs^{(m)}(x)$ from which the total recombination coefficient to all levels

$$\alpha_t = \sum_{p'=1}^{\infty} \alpha_{p'} \quad (A-28)$$

may be calculated directly.

For more complex systems the only method generally applicable is an extension of the Coulomb approximation. This yields formulas identical to (A-16) and (A-17) except that n is replaced by an effective quantum number $n^* = z/\sqrt{I_{nl}}$, z being the residual charge on the atom when the electron has been ejected.

TABLE A-5
RADIATIVE RECOMBINATION COEFFICIENTS $\alpha(P/T_e)$ FOR HYDROGEN IN cm^3/sec

T_e °K	250	500	1000	2000	4000	8000	16000	32000	64000
P									
1	$1.015 \cdot 10^{-12}$	$7.168 \cdot 10^{-13}$	$5.068 \cdot 10^{-13}$	$3.563 \cdot 10^{-13}$	$2.500 \cdot 10^{-13}$	$1.740 \cdot 10^{-13}$	$1.196 \cdot 10^{-13}$	$8.024 \cdot 10^{-14}$	$5.190 \cdot 10^{-14}$
2	$5.662 \cdot 10^{-13}$	$3.985 \cdot 10^{-13}$	$2.787 \cdot 10^{-13}$	$1.937 \cdot 10^{-13}$	$1.323 \cdot 10^{-13}$	$8.804 \cdot 10^{-14}$	$5.631 \cdot 10^{-14}$	$3.419 \cdot 10^{-14}$	$1.952 \cdot 10^{-14}$
3	$3.896 \cdot 10^{-13}$	$2.723 \cdot 10^{-13}$	$1.884 \cdot 10^{-13}$	$1.279 \cdot 10^{-13}$	$8.438 \cdot 10^{-14}$	$5.331 \cdot 10^{-14}$	$3.189 \cdot 10^{-14}$	$1.799 \cdot 10^{-14}$	$9.459 \cdot 10^{-15}$
4	$2.952 \cdot 10^{-13}$	$2.045 \cdot 10^{-13}$	$1.393 \cdot 10^{-13}$	$9.233 \cdot 10^{-14}$	$5.864 \cdot 10^{-14}$	$3.532 \cdot 10^{-14}$	$2.001 \cdot 10^{-14}$	$1.063 \cdot 10^{-14}$	$5.301 \cdot 10^{-15}$
5	$2.362 \cdot 10^{-13}$	$1.619 \cdot 10^{-13}$	$1.084 \cdot 10^{-13}$	$6.992 \cdot 10^{-14}$	$4.292 \cdot 10^{-14}$	$2.481 \cdot 10^{-14}$	$1.346 \cdot 10^{-14}$	$6.875 \cdot 10^{-15}$	$3.320 \cdot 10^{-15}$
6	$1.957 \cdot 10^{-13}$	$1.326 \cdot 10^{-13}$	$8.701 \cdot 10^{-14}$	$5.476 \cdot 10^{-14}$	$3.256 \cdot 10^{-14}$	$1.818 \cdot 10^{-14}$	$9.533 \cdot 10^{-15}$	$4.714 \cdot 10^{-15}$	$2.219 \cdot 10^{-15}$
7	$1.660 \cdot 10^{-13}$	$1.111 \cdot 10^{-13}$	$7.163 \cdot 10^{-14}$	$4.394 \cdot 10^{-14}$	$2.539 \cdot 10^{-14}$	$1.377 \cdot 10^{-14}$	$7.021 \cdot 10^{-15}$	$3.391 \cdot 10^{-15}$	$1.563 \cdot 10^{-15}$
8	$1.432 \cdot 10^{-13}$	$9.462 \cdot 10^{-14}$	$5.991 \cdot 10^{-14}$	$3.591 \cdot 10^{-14}$	$2.023 \cdot 10^{-14}$	$1.069 \cdot 10^{-14}$	$5.337 \cdot 10^{-15}$	$2.526 \cdot 10^{-15}$	$1.145 \cdot 10^{-15}$
9	$1.253 \cdot 10^{-13}$	$8.170 \cdot 10^{-14}$	$5.081 \cdot 10^{-14}$	$2.981 \cdot 10^{-14}$	$1.642 \cdot 10^{-14}$	$8.506 \cdot 10^{-15}$	$4.158 \cdot 10^{-15}$	$1.934 \cdot 10^{-15}$	$8.660 \cdot 10^{-16}$
10	$1.108 \cdot 10^{-13}$	$7.126 \cdot 10^{-14}$	$4.358 \cdot 10^{-14}$	$2.507 \cdot 10^{-14}$	$1.353 \cdot 10^{-14}$	$6.881 \cdot 10^{-15}$	$3.310 \cdot 10^{-15}$	$1.519 \cdot 10^{-15}$	$6.722 \cdot 10^{-16}$
11	$9.876 \cdot 10^{-14}$	$6.270 \cdot 10^{-14}$	$3.772 \cdot 10^{-14}$	$2.132 \cdot 10^{-14}$	$1.131 \cdot 10^{-14}$	$5.654 \cdot 10^{-15}$	$2.682 \cdot 10^{-15}$	$1.217 \cdot 10^{-15}$	$5.291 \cdot 10^{-16}$
12	$8.866 \cdot 10^{-14}$	$5.558 \cdot 10^{-14}$	$3.292 \cdot 10^{-14}$	$1.831 \cdot 10^{-14}$	$9.533 \cdot 10^{-15}$	$4.708 \cdot 10^{-15}$	$2.207 \cdot 10^{-15}$	$9.8899 \cdot 10^{-16}$	$4.298 \cdot 10^{-16}$
$\int \alpha(P) \cdot P^{-1}$	$4.842 \cdot 10^{-12}$	$3.117 \cdot 10^{-12}$	$1.988 \cdot 10^{-12}$	$1.257 \cdot 10^{-12}$	$7.850 \cdot 10^{-13}$	$4.833 \cdot 10^{-13}$	$2.926 \cdot 10^{-13}$	$1.734 \cdot 10^{-13}$	$1.002 \cdot 10^{-13}$

The indices give the powers of 10 by which the entries must be multiplied.

According to Burgess and Seaton^(A-16)

$$g(n^* \ell; \epsilon' \ell') = \frac{G(n^* \ell; \epsilon' \ell')}{\zeta^{\frac{1}{2}}(n^*, \ell)} \cos \pi [n^* + \mu(\epsilon') + \chi(n^* \ell; \epsilon' \ell')] \quad (A-29)$$

where

$$G(n^* \ell; \epsilon' \ell') = \frac{(-1)^{\ell+1} G_{\ell \ell'}(n^*)}{(1+\epsilon' n^*)^2 Y_{\ell \ell'}(n^*)} \quad (A-30)$$

and

$$\chi(n^* \ell; \epsilon' \ell') = \chi_{\ell \ell'}(n^*) + \frac{\epsilon' n^*}{1+\epsilon' n^*} \alpha_{\ell \ell'} + \frac{\epsilon' n^{*2}}{1+\epsilon' n^*} \beta_{\ell \ell'}(n^*) \quad (A-31)$$

$\mu(\epsilon')$ is the continuum phase shift obtained by extrapolation of the quantum defects $\mu(I_{n \ell})$ of the energy levels of the bound states.

$$\zeta(n^*, \ell) = 1 + \frac{2}{n^*} \frac{\partial \chi(\epsilon)}{\partial \epsilon} \quad (A-32)$$

and

$$\chi_{\ell \ell'}(n^*) = a_{\ell \ell'} + \frac{b_{\ell \ell'}}{n^*} - \frac{c_{\ell \ell'}}{n^{*2}} \quad (n^* \geq \ell + 2) \quad (A-33)$$

The remaining functions $G_{\ell \ell'}(n^*)$, $\chi_{\ell \ell'}(n^*)$ and coefficients $a_{\ell \ell'}$, $b_{\ell \ell'}$, $c_{\ell \ell'}$, $\alpha_{\ell \ell'}$, $\beta_{\ell \ell'}$, have been tabulated by Burgess and Seaton for $1 \leq n^* \leq 12$ and $\ell, \ell' \leq 3$. For values of $n^* < \ell + 2$, additional tables are presented which permit the calculation of $g(n^* \ell; \epsilon' \ell')$ for transitions from specific bound states to the continuum.

As an example of the application of Burgess and Seaton's^(A-16) formulas and tables to the treatment of complex atomic systems, they have been used to calculate the photoionization cross sections and radiative recombination coefficients for some of the observed states of aluminum. The ground state configuration of Al I is $3s^2 3p$ and the observed excited

states, with the exception of one $3s3p^2$ configuration, are configurations of the form $3s^2 n\ell$ where $3 \leq n \leq 11$ and $0 \leq \ell \leq 3$ (cf. C. Moore^(A-17)). The latter configurations consist of a single ($n\ell$) electron outside a closed shell for which the C_ℓ , assume the particularly simple form (selection rules on the azimuthal quantum number allow only transitions where $\ell' = \ell \pm 1$):

$$C_{\ell+1} = \frac{\ell+1}{2\ell+1} \quad , \quad C_{\ell-1} = \frac{\ell}{2\ell+1} \quad (A-34)$$

Table A-6 gives the Burgess and Seaton coefficients for the allowed transitions in Al I. These coefficients were used to calculate the functional parameters $\chi_{\ell\ell}, (n^*)$, $G_{\ell\ell}, (n^*)$, $\gamma_{\ell\ell}, (n^*)$ for individual transitions. The results, together with the ionization potentials and quantum defects of the bound states $\mu(-I_{n\ell})$, are listed in Table A-7. The $\zeta(n^*, \ell)$, also given in Table A-7, were determined from the curves of Figure A-1 which shows plots of the continuous phase shifts for each ($n\ell$) series.

For small positive electron energies ϵ' , the phase shift may be taken as a linear function of ϵ' . The extrapolated quantum defects determined from the curves of Figure A-1, lead to the following approximate expressions for $\mu(\epsilon')$:

$$\mu(\epsilon') = 1.755 \quad (\text{ns series})$$

$$\mu(\epsilon') = 1.264 - 0.065\epsilon' \quad (\text{np series}) \quad (A-35)$$

$$\mu(\epsilon') = 0.985 + 3.3\epsilon' \quad (\text{nd series})$$

$$\mu(\epsilon') = 0.044 + 0.26\epsilon' \quad (\text{nf series})$$

TABLE A-6
PARAMETERS FOR CALCULATION OF AI I PHOTIONIZATION CROSS SECTIONS

Transition	$a_{II'}$	$b_{II'}$	$c_{II'}$	$\alpha_{II'}$	$\beta_{II'*}$	$c_{I'}$
ns - $\epsilon' p$	-0.147	+0.2515	-0.0780	0.310	0.000	1
np - $\epsilon' s$	-0.216	-0.171	0.000	0.000	0.000	1/3
np - $\epsilon' d$	-0.120	+0.600	0.000	0.362	0.0535	2/3
nd - $\epsilon' p$	-0.247	-0.272	0.000	-0.010	-0.019	2/5
nd - $\epsilon' f$	0.117	+1.170	0.000	+0.321	+0.106	3/5
nf - $\epsilon' d$	-0.362	+0.599	-2.432	-0.390	+0.0500	3/7

Note for 3p - $\left\{ \begin{array}{l} \epsilon' s \\ \epsilon' d \end{array} \right\}$ $\beta_{12}(n) = 0.046$

TABLE A-7
PARAMETERS FOR CALCULATION OF AI I PHOTOIONIZATION CROSS SECTIONS

Transition	$I_{n\ell}$	n^*	$\mu(-I_{n\ell})$	$\xi(n^*, \ell)$	$\chi_{II^*}(n^*)$	$G_{II^*}(n^*)$	$\gamma_{II^*}(n^*)$
$4s - e'p$	0.2091	2.187	1.813	0.9116	-0.0483	2.050	1.602
$5s - e'p$.09655	3.218	1.781	0.9938	-0.0764	1.826	1.591
$6s - e'p$.05593	4.228	1.772	1.000	-0.0919	1.696	1.590
$7s - e'p$.03652	5.233	1.767	1.000	-0.1018	1.607	1.592
$8s - e'p$.02573	6.234	1.766	1.000	-0.1087	1.540	1.595
$9s - e'p$.01910	7.236	1.764	1.000	-0.1137	1.487	1.597
$10s - e'p$.01471	8.245	1.755	1.000	-0.1176	1.443	1.599
$3p - e's$							
$3p - e'd$.44019	1.507	1.507	0.9809	-0.3095	0.868	1.609
$4p - e's$.13977	2.675	1.324	0.9785	+0.3380	3.232	1.674
$4p - e'd$.13977	2.675	1.324	0.9785	-0.2799	1.078	1.667
$5p - e's$.07301	3.701	1.299	0.9615	+0.1043	2.452	1.578
$5p - e'd$.07301	3.701	1.299	0.9615	0.0422	1.309	1.667
$6p - e's$.04508	4.710	1.290	0.9980	-0.2622	1.901	1.580
$6p - e'd$.04508	4.710	1.290	0.9980	+0.0074	1.163	1.667
$7p - e's$.03055	5.721	1.279	0.9947	-0.2523	1.901	1.581
$7p - e'd$.03055	5.721	1.279	0.9947	-0.0151	1.779	1.586
$3d - e'p$							
$3d - e'f$.14446	2.621	0.379	1.328	(-0.3508)	(0.660)	(1.820)
$4d - e'p$.08525	3.423	0.379	1.328	(+0.3294)	(3.100)	(1.440)
$4d - e'f$.08525	3.423	0.577	1.180	(-0.3265)	(0.732)	(1.799)
$5d - e'p$.05512	4.259	0.577	1.180	(+0.2248)	(2.752)	(1.484)
$5d - e'f$.05512	4.259	0.721	1.179	-0.3109	0.839	1.763
					+0.1577	2.342	1.537

TABLE A -7 (continued)

Transition	I_{nl}	n^*	$\mu(-I_{nl})$	$\zeta(n^*, l)$	$\chi_{LL'}(n^*)$	$G_{LL'}(n^*)$	$\gamma_{LL'}(n^*)$
6d - $\epsilon' p$.03750	5.164	0.836	1.067	-0.2997	0.908	1.738
6d - $\epsilon' f$.03750	5.164	0.836	1.067	+0.1096	2.112	1.545
7d - $\epsilon' p$.02676	6.113	0.887	1.041	-0.2915	0.956	1.720
7d - $\epsilon' f$.02676	6.113	0.887	1.041	+0.0744	1.958	1.550
8d - $\epsilon' p$.01992	7.084	0.916	1.021	-0.2854	0.990	1.706
8d - $\epsilon' f$.01992	7.084	0.916	1.021	+0.0482	1.847	1.557
9d - $\epsilon' p$.01537	8.066	0.934	1.014	-0.2807	1.015	1.696
9d - $\epsilon' f$.01537	8.066	0.934	1.014	+0.0281	1.760	1.565
10d - $\epsilon' p$.01219	9.050	0.940	1.010	-0.2770	1.034	1.688
10d - $\epsilon' f$.01219	9.060	0.940	1.010	+0.0121	1.695	1.573
11d - $\epsilon' p$.00991	10.044	0.956	1.007	-0.2741	1.047	1.682
11d - $\epsilon' f$.00991	10.044	0.956	1.007	-0.0005	1.633	1.581
4f - $\epsilon' d$.06346	3.970	0.030	1.001	-0.3654	0.468	1.850
5f - $\epsilon' d$.04056	4.966	0.034	1.000	-0.3400	0.595	1.906
6f - $\epsilon' d$.02812	5.963	0.037	1.000	-0.3309	0.700	1.918
7f - $\epsilon' d$.02064	6.961	0.039	1.000	-0.3262	0.790	1.920

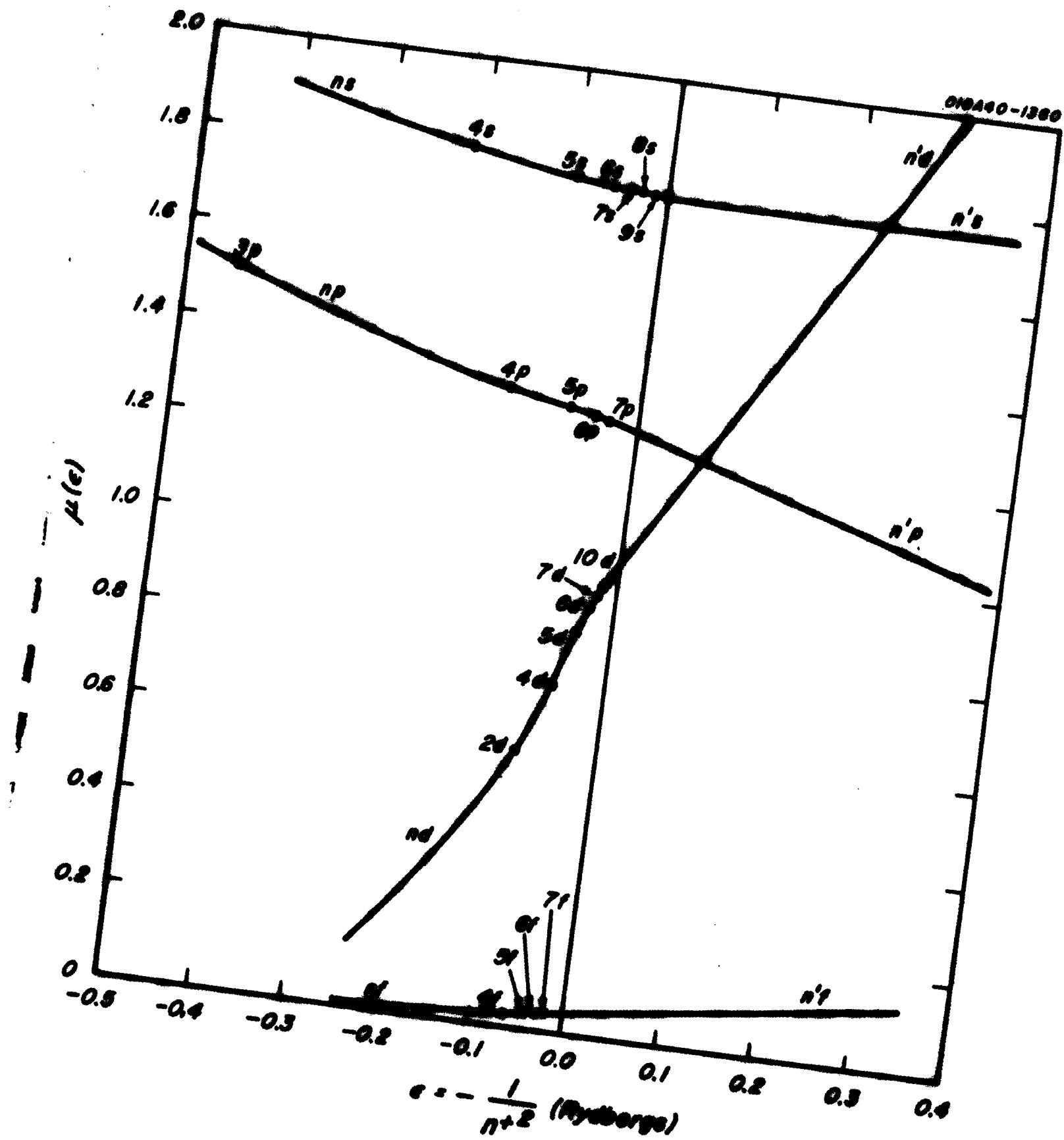


Figure A-1. Quantum Defects and Continuum Phase Shifts Obtained From Al I Energy Levels.

Photoionization cross sections were calculated for all but the $3s3p^2$ and nf levels, for ejected electron energies ϵ' lying in the interval (Rydbergs) $0 \leq \epsilon' \leq 0.5$ for the nd levels, $0 \leq \epsilon' \leq 0.3$ for the ns levels and $0 \leq \epsilon' \leq 0.2$ for the np series. For electron energies in excess of the maximum values indicated, it was found that the approximate formulas led to incorrect results. This may in part be due to the assumption of a linear dependence for the $\mu(\epsilon')$; however, it should be noted that the approximations inherent in the derivation of (A-29) limit the validity of the calculations to small ejected electron energies.

The photoionization cross sections obtained are listed in Table A-8. The $3s^23d$ and $3s^24d$ cross sections were calculated under the assumption that $n^* \geq l+2$ since explicit expressions are not tabulated by Burgess and Seaton^(A-16) for $nd \rightarrow \epsilon'p$ and $nd \rightarrow \epsilon'f$ transitions when $n^* < l+2$. The resulting cross sections are therefore of lesser accuracy than the remaining cross sections shown.

The radiative recombination coefficient may be calculated from Eq. (A-12) once the photoionization cross sections are known as functions of the ejected electron energy. Thus, in terms of electron energy for a thin plasma

$$\alpha(nl|T_e) = \frac{1}{c} \frac{1}{2} \left(\frac{2}{\pi} \right)^{\frac{1}{2}} \frac{2(2l+1)}{(mkT_e)^{3/2}} \int_0^{\infty} Q_v(nl)(I_{nl} + \epsilon)^2 e^{-\epsilon/kT_e} d\epsilon \quad (A-36)$$

Instead of evaluating the integral of (A-36), the recombination coefficient can be determined approximately by use of the expression

$$\alpha(nl|T_e) = \bar{v} Q_{\bar{\epsilon}}(nl) \quad (A-37)$$

TABLE A-8
PROTONIZATION CROSS SECTIONS FOR Al I ($Q_\nu(n\mu) \times 10^{19}$) IN cm^2

where $Q_\epsilon (nl)$ the cross section for radiative recombination is given by detailed balancing

$$Q_\epsilon (nl) = (2\ell+1) \frac{(I_{p\ell} + \epsilon)^2}{mc^2 \epsilon} Q_\nu (nl) \quad (A-38)$$

and \bar{v} is the average electron speed

$$\bar{v} = \left(\frac{8kT_e}{m} \right)^{1/2} \quad (A-39)$$

Substituting (A-39) and (A-38) in (A-37), we find

$$\begin{aligned} \alpha(n\ell | T_e) &= \left(\frac{m}{8kT_e} \right)^{1/2} \frac{2(2\ell+1)}{mc^2} (I_p + \epsilon)^2 Q_\nu (nl) \\ &= 2.046 \times 10^6 (2\ell+1) (I_p + \epsilon)^2 \frac{Q_\nu (nl)}{T_e^{1/2}} \end{aligned} \quad (A-40)$$

The radiative recombination coefficients calculated from (A-40) are given in Table A-9 for electron temperatures of 6190°K and $24,760^\circ\text{K}$.

TABLE A-9

RADIATIVE RECOMBINATION COEFFICIENTS
 FOR Al I $\alpha(n\ell|T_e) \text{ in cm}^3/\text{sec}$

 $T_e = 6190^\circ\text{K}$ $T_e = 24,760^\circ\text{K}$

$n \backslash \ell$	s	p	d		s	p	d
3		2.11(-13)	6.48(-14)			8.04(-15)	1.94(-14)
4	9.80(-15)	3.90(-14)	2.36(-14)		1.99(-16)	1.73(-15)	1.53(-14)
5	1.86(-16)	1.32(-14)	1.04(-16)		5.34(-17)	7.68(-16)	2.56(-15)
6	7.28(-16)	5.62(-15)	9.39(-16)		9.24(-17)	2.68(-16)	6.80(-16)
7	4.94(-16)	5.06(-15)	1.33(-15)		1.01(-16)	2.96(-16)	2.21(-16)
8	1.74(-17)		1.28(-14)		8.35(-17)		1.31(-16)
9	8.35(-18)		1.10(-16)		7.63(-17)		1.03(-16)
10	2.22(-18)		8.66(-16)		8.04(-17)		8.46(-16)
11			7.33(-16)				7.52(-16)

The brackets give the power of 10 by which the entries must be multiplied.

A.3 Electron Collision Induced Transitions Between Bound States

Let $q_\epsilon(p, q)$ be the cross section for the excitation to the q state by the impact of an electron of energy ϵ with an atom in the p state.

The rate of depopulation of the p^{th} state by electron impact is

$$n_e n(p) \sum_{r > p} C(p, r) \quad (\text{A-41})$$

where the collision probability $C(p, r)$ depends upon the electron temperature T_e and is obtained by integrating the product of the electron velocity and the cross section over the Maxwellian distribution according to

$$C(p, r) = \left(\frac{8}{\pi m} \right)^{1/2} (kT_e)^{-3/2} \int_{-\infty}^{\infty} q_\epsilon(p, r) \epsilon \exp(-\epsilon/kT_e) d\epsilon \quad (\text{A-42})$$
$$I_r = I_p$$

The probability of de-excitation to a lower level is similarly

$$n_e n(p) \sum_q C(p, q) \quad (\text{A-43})$$

The direct and inverse collision probabilities are related through the principle of detailed balancing:

$$C(p,q) = \frac{\omega_q}{\omega_p} \exp \left\{ \frac{I_q - I_p}{kT} \right\} C(q,p) \quad (A-44)$$

The p^{th} state may also be populated by electron impact induced excitation and de-excitation and the appropriate rates are

$$n_e \sum_{q < p} n(q) C(q,p) \quad (A-45)$$

$$n_e \sum_{r > p} n(r) C(r,p) \quad (A-46)$$

There are various simple ways of computing the probabilities of excitation and de-excitation transitions induced by electron-atom collisions (c.f. Allen^(A-4)), none of which is entirely satisfactory. Those quantum mechanical treatments in which some reliability may be placed (e.g. Mott and Massey^(A-18), Bates et al^(A-19), Milford and co-workers^(A-20), McCrea and Mc Kirgan^(A-21), and Mc Carroll^(A-22) have been based on the Born approximation, and therefore, are valid only for high electron impact energies.

A simplified formula describing the cross-section for excitation from a q level to a p level induced by the form (c.f. Allen^(A-4))

$$Q_{\epsilon}(q,p) = 1.44 \times 10^{11} \pi a_0^2 (ch)^2 f(q,p) \frac{1}{\epsilon} \left(\frac{1}{\epsilon_{q,p}} - \frac{1}{\epsilon} \right) \text{ cm}^2 \quad (A-47)$$

where ϵ denotes the impacting electron energy, and $\epsilon_{q,p}$ is the excitation energy, both expressed in Rydbergs ($\epsilon_{q,p} = \epsilon_q - \epsilon_p$). $f(q,p)$ represents the oscillator strength for absorption, and is related to the spontaneous transition probability $A(p,q)$ by

$$f(q,p) = \frac{mc^3}{8\pi \epsilon^2 \nu} \frac{\omega_p}{\omega_q} A(p,q) \quad (A-48)$$

Equations (A-47) and (A-48) may be used to calculate collisional transition probabilities for the atomic systems for which the spontaneous transition probabilities are given in Tables A-1, A-2, and A-3. If $Q_{\epsilon}(p,q)$ denotes the corresponding collisional de-excitation cross section, then (A-47) and (A-48), with the aid of the following expression (c.f. Allen^(A-4)):

$$\omega_q \epsilon_p Q_{\epsilon}(p,q) = \omega_q \epsilon_q Q_{\epsilon}(q,p) \quad (A-49)$$

$$\omega_p f(p,q) = \omega_q f(q,p) \quad (A-50)$$

yields

$$Q_{\epsilon}(p,q) = 5.78 \times 10^{11} \pi a_0^2 (ch)^2 \frac{\omega_q}{\omega_p} f(q,p) \left(\frac{\epsilon_q}{\epsilon_p} \right) \quad (A-51)$$

Expressions similar to (A-47) and (A-51) with values of $A(p,q)$ obtained by the formulas of Menzel and Pekeris^(A-7) for hydrogen were employed by Giovanelli^(A-10) and Ivanov-Kholodnyi et al^(A-13).

Perhaps the most accurate method of computing collisional transition probabilities is the classical method of Gryzinski (A-23), which represents an improvement over the original formulation of Thomson (A-24), in that it takes account of the fact that the atomic electrons are moving. The cross-sections so desired fall off too rapidly at high electron energies, as ϵ^{-1} instead of the correct $(\epsilon^{-1} \ln \epsilon)$, but their accuracy probably suffices, the effect of excitation and de-excitation not being a primary one.

Considering in some detail the classical transfer of momentum during a coulomb collision between an incident electron of energy ϵ and an atomic electron having binding energy ϵ_p , Gryzinski derived the following approximate expression for the differential cross-section $\sigma(\Delta\epsilon)$ corresponding to a loss in energy of the incident electron of magnitude $\Delta\epsilon$:

$$\sigma(\Delta\epsilon) \approx \frac{\pi e^4}{\epsilon(\Delta\epsilon)^2} \left(\frac{\epsilon}{\epsilon + \epsilon_p} \right)^{3/2} \begin{cases} 1 - \frac{\epsilon_p}{\epsilon} + \frac{4}{3} \frac{\epsilon_p}{\Delta\epsilon} & \Delta\epsilon \leq \epsilon - \epsilon_p \\ \frac{1}{3} \left[1 + 4 \frac{\epsilon_p}{\Delta\epsilon} + 2 \frac{\Delta\epsilon}{\epsilon} - \frac{\epsilon_p}{\epsilon} \right] \left[\left(1 + \frac{\Delta\epsilon}{\epsilon_p} \right) \left(1 - \frac{\Delta\epsilon}{\epsilon} \right) \right]^{1/2} & \Delta\epsilon \geq \epsilon - \epsilon_p \end{cases} \quad (A-52)$$

The total cross section for a collision involving an energy loss $\Delta\epsilon$ subject to the restriction $\epsilon_p \leq \epsilon \leq \epsilon_q$ is then given by

$$Q_\epsilon(\epsilon_p, \epsilon_q) = \int_{\epsilon_q}^{\epsilon_p} \sigma(\Delta\epsilon) d(\Delta\epsilon) = Q(\epsilon_p) - Q(\epsilon_q) \quad (A-53)$$

where $Q(\epsilon_p)$ the cross section for a collision with electron loss greater than ϵ_p is defined by Equation (A-45). Thus when $\Delta\epsilon = \epsilon_p$, as in the case for hydrogenic orbits,

$$Q(\epsilon_p) = \frac{3.55 \times 10^{-16}}{\epsilon_p^2} \left(\frac{\epsilon}{\epsilon + \epsilon_p} \right)^{3/2} \begin{cases} \frac{2}{3} \frac{\epsilon_p}{\epsilon} + \frac{\epsilon_p}{\epsilon} \left(1 - \frac{\epsilon_p}{\epsilon} \right) - \left(\frac{\epsilon_p}{\epsilon} \right)^2 \text{ (cm}^2\text{)} & 2\epsilon_p \leq \epsilon \\ \frac{2}{3} \left[\frac{\epsilon_p}{\epsilon} + \frac{\epsilon_p}{\epsilon} \left(1 - \frac{\epsilon_p}{\epsilon} \right) - \left(\frac{\epsilon_p}{\epsilon} \right)^2 \right] \\ \times \left(1 - \frac{\epsilon_p}{\epsilon} \right)^{1/2} \text{ (cm}^2\text{)} & 2\epsilon_p \geq \epsilon \end{cases} \quad (A-54)$$

The collision transition probability is given by

$$C(p, q) = \left(\frac{8}{\pi m} \right)^{1/2} (kT_e)^{-3/2} \int_0^\infty Q_e(\epsilon_q; \epsilon_p) \epsilon e^{-\epsilon/kT_e} e_d \epsilon \quad (A-55)$$

Inserting $Q_e(\epsilon_q; \epsilon_p)$ leads to the following collision probabilities for hydrogen, where $\epsilon_p = 1/p^2$ and $\epsilon_p = 1/q^2$

$$C(p, q) = \frac{10.9}{T_e^{3/2}} \frac{g_0^2}{q^3} \int_1^\infty \xi \exp \left\{ \frac{-1.5789 \times 10^5}{q p^2 T_e} y \right\} dy \text{ cm}^3 \text{ sec}^{-1} \quad (A-56)$$

where

$$g = \frac{q^2}{(q^2 - p^2)} \quad y = \epsilon_p^2 g \quad (A-57)$$

and

$$\xi = \begin{cases} \frac{\frac{1}{3} [2 - (g + y(1 + 4g))] (y - 1)^{1/2} (g + 1)^{1/2}}{g^{1/2} (g + y)^{3/2}} & y < 1 + g \\ \frac{\frac{1}{3} [-3g + y(3 + 4g)] y^{1/2}}{(g + y)^{3/2}} & y > 1 + g \end{cases} \quad (A-58)$$

$$\xi = \begin{cases} \frac{\frac{1}{3} [-3g + y(3 + 4g)] y^{1/2}}{(g + y)^{3/2}} & y > 1 + g \end{cases} \quad (A-59)$$

$C(p, q)$ has been calculated for hydrogen by Bates using equation (A-56). The results are given in Table (A-10) for $p & q$ less than or equal to 10.

TABLE A-10
CONVENTIONAL EXCITATION AND DE-EXCITATION, COEFFICIENTS FOR HYDROGEN $c(p,q)$ IN cm^3/sec

		$T_e = 250^\circ\text{K}$											$T_e = 300^\circ\text{K}$										
		p											q										
		1	2	3	4	5	6	7	8	9	10	11	1	2	3	4	5	6	7	8	9	10	11
1	-	6.9(-214)	1.2(-252)	2.1(-266)	6.8(-273)	1.7(-276)	1.0(-278)	3.3(-280)	2.8(-281)	4.7(-282)	1.2(-282)		4.9(-111)	9.2(-131)	7.5(-138)	3.0(-141)	3.6(-143)	2.2(-144)	3.2(-145)	7.9(-146)	2.7(-146)	1.2(-146)	
2	8.6(-9)	-	4.8(-45)	5.2(-59)	1.4(-65)	3.3(-69)	1.8(-71)	5.7(-73)	5.0(-74)	8.1(-75)	2.0(-75)		8.6(-9)	-	5.4(-26)	4.3(-30)	2.2(-32)	6.5(-34)	5.3(-35)	8.5(-36)	2.0(-36)		
3	8.0(-10)	2.6(-7)	-	1.5(-19)	2.3(-26)	4.3(-30)	2.2(-32)	7.3(-16)	2.9(-18)	7.7(-20)	6.0(-21)	9.0(-22)	2.1(-22)		8.0(-10)	2.7(-7)	6.7(-6)	-	1.2(-8)	2.6(-11)	5.4(-13)	3.7(-14)	5.2(-15)
4	1.7(-10)	3.4(-8)	1.7(-6)	-	7.0(-12)	7.3(-16)	2.9(-18)	7.7(-11)	5.4(-13)	3.7(-14)	1.1(-15)												
5	5.3(-11)	9.0(-9)	2.7(-7)	6.7(-6)	-	1.2(-8)	2.6(-11)	5.4(-13)	3.7(-14)	5.2(-15)	1.1(-15)												
6	2.1(-11)	3.2(-9)	7.3(-8)	1.1(-6)	1.9(-5)	-	5.8(-7)	6.2(-9)	3.3(-10)	4.1(-11)	8.4(-12)												
7	9.6(-12)	1.4(-9)	3.0(-8)	3.4(-7)	3.2(-6)	4.5(-5)	-	6.0(-6)	1.6(-7)	1.5(-8)	2.7(-9)												
8	4.9(-12)	6.9(-10)	1.4(-8)	1.4(-7)	1.0(-6)	7.6(-6)	9.5(-5)	-	3.0(-5)	1.4(-6)	1.9(-7)												
9	2.7(-12)	3.7(-10)	7.3(-9)	6.7(-8)	4.4(-7)	2.5(-6)	1.6(-5)	1.8(-4)	-	9.6(-5)	6.2(-6)												
10	1.6(-12)	2.1(-10)	4.1(-9)	3.6(-8)	2.2(-7)	1.1(-6)	5.3(-6)	3.0(-5)	3.4(-4)	-	2.4(-4)												

The brackets give the powers of 10 by which the entries must be multiplied.

TABLE A-10 (continued)

 $T_e = 1000^\circ K$

p	q	1	2	3	4	5	6	7	8	9	10	11
1	-	1.3(-59)	8.1(-70)	1.4(-73)	2.0(-75)	1.6(-76)	3.2(-77)	9.9(-78)	4.1(-78)	2.0(-78)	1.2(-78)	
2	8.6(-9)	-	1.8(-16)	1.9(-20)	2.2(-22)	1.7(-23)	3.1(-24)	9.4(-25)	3.8(-25)	1.8(-25)	1.1(-25)	
3	8.1(-10)	2.7(-7)	-	1.5(-9)	1.0(-11)	6.1(-13)	1.0(-13)	2.8(-14)	1.1(-14)	5.4(-15)	3.0(-15)	
4	1.7(-10)	3.5(-8)	1.9(-6)	-	3.4(-7)	1.1(-8)	1.4(-9)	3.5(-10)	1.3(-10)	5.8(-11)	3.1(-11)	
5	5.4(-11)	9.0(-9)	2.7(-7)	7.6(-6)	-	4.8(-6)	3.1(-7)	6.0(-8)	1.9(-8)	7.9(-9)	4.0(-9)	
6	2.1(-11)	3.2(-9)	7.9(-8)	1.1(-6)	2.3(-5)	-	2.5(-5)	2.3(-6)	5.4(-7)	2.0(-7)	9.1(-8)	
7	9.6(-12)	1.4(-9)	3.1(-8)	3.5(-7)	3.5(-6)	5.9(-5)	-	8.0(-5)	8.8(-6)	2.4(-6)	9.4(-7)	
8	4.9(-12)	6.9(-10)	1.4(-8)	1.4(-7)	1.1(-6)	8.7(-6)	1.3(-4)	-	2.0(-4)	2.4(-5)	7.0(-6)	
9	2.7(-12)	3.7(-10)	7.3(-9)	6.9(-8)	4.6(-7)	2.7(-6)	1.9(-5)	2.7(-4)	-	4.2(-4)	5.4(-5)	
10	1.6(-12)	2.1(-10)	4.1(-9)	3.7(-8)	2.3(-7)	1.2(-6)	6.0(-6)	3.8(-5)	4.9(-4)	-	7.9(-4)	

 $T_e = 2000^\circ K$

p	q	1	2	3	4	5	6	7	8	9	10	11
1	-	6.9(-34)	2.5(-39)	2.0(-41)	1.7(-42)	3.6(-43)	1.3(-43)	5.8(-44)	3.1(-44)	1.9(-44)	1.2(-44)	
2	8.6(-9)	-	1.1(-11)	5.3(-14)	3.6(-15)	7.1(-16)	2.3(-16)	1.0(-16)	5.4(-17)	3.2(-17)	2.1(-17)	
3	8.1(-10)	2.8(-7)	-	7.7(-8)	2.9(-9)	4.5(-10)	1.3(-10)	5.4(-11)	2.7(-11)	1.6(-11)	1.0(-11)	
4	1.7(-10)	3.5(-8)	2.0(-6)	-	2.2(-6)	1.7(-7)	4.0(-8)	1.4(-8)	6.7(-9)	3.7(-9)	2.3(-9)	
5	5.4(-11)	9.1(-9)	2.8(-7)	8.5(-6)	-	1.4(-5)	1.6(-5)	4.3(-7)	1.7(-7)	8.7(-8)	5.0(-8)	
6	2.1(-11)	3.3(-9)	8.1(-8)	1.2(-6)	2.6(-5)	-	5.2(-5)	6.4(-6)	1.9(-6)	8.3(-7)	4.4(-7)	
7	9.6(-12)	1.4(-9)	3.1(-8)	3.6(-7)	3.7(-6)	6.8(-5)	-	1.3(-4)	1.8(-5)	5.7(-6)	2.5(-6)	
8	4.9(-12)	6.9(-10)	1.4(-8)	1.4(-7)	1.1(-6)	9.5(-6)	1.5(-4)	-	2.9(-4)	4.1(-5)	1.3(-5)	
9	2.7(-12)	3.7(-10)	7.4(-9)	7.0(-8)	4.7(-7)	2.9(-6)	2.1(-5)	3.0(-4)	-	5.6(-4)	8.0(-5)	
10	1.6(-12)	2.1(-10)	4.2(-9)	3.7(-8)	2.3(-7)	1.2(-6)	6.3(-6)	4.1(-5)	5.5(-4)	-	9.9(-4)	

The brackets give the powers of 10 by which the entries must be multiplied.

TABLE A-10 (continued)

		$T_e = 4000^{\circ}\text{K}$										
		1	2	3	4	5	6	7	8	9	10	11
P	q	1	2	3	4	5	6	7	8	9	10	11
1	-	4.9(-21)	4.3(-24)	2.4(-25)	4.8(-26)	1.6(-26)	7.7(-27)	4.3(-27)	2.6(-27)	1.7(-27)	1.2(-27)	
2	8.7(-9)	-	2.7(-9)	8.8(-11)	1.4(-11)	4.6(-12)	2.0(-12)	1.1(-12)	6.4(-13)	4.2(-13)	2.9(-13)	
3	0.1(-10)	2.9(-7)	-	5.7(-7)	4.9(-8)	1.2(-8)	4.8(-9)	2.4(-9)	1.4(-9)	8.6(-10)	5.8(-10)	
4	1.7(-10)	3.6(-8)	2.2(-6)	-	6.0(-6)	7.3(-7)	2.2(-7)	9.4(-8)	4.9(-8)	2.9(-8)	1.9(-8)	
5	5.4(-11)	9.2(-9)	2.9(-7)	9.4(-6)	-	2.6(-5)	3.6(-6)	1.1(-6)	5.2(-7)	2.8(-7)	1.7(-7)	
6	2.1(-11)	3.3(-9)	8.3(-8)	1.3(-6)	2.9(-5)	-	7.6(-5)	1.1(-5)	3.6(-6)	1.7(-6)	9.4(-7)	
7	9.6(-12)	1.4(-9)	3.2(-8)	3.7(-7)	4.0(-6)	7.5(-5)	-	1.8(-4)	2.6(-5)	8.7(-6)	4.1(-6)	
8	4.9(-12)	7.0(-10)	1.4(-8)	1.5(-7)	1.2(-6)	9.9(-6)	1.6(-4)	-	3.5(-4)	5.2(-5)	1.7(-5)	
9	2.7(-12)	3.7(-10)	7.5(-9)	7.1(-8)	4.8(-7)	3.0(-6)	2.1(-5)	3.1(-4)	-	6.3(-4)	9.3(-5)	
10	1.6(-12)	2.2(-10)	4.2(-9)	3.7(-8)	2.3(-7)	1.2(-6)	6.4(-6)	4.1(-5)	5.6(-4)	-	1.0(-3)	

		$T_e = 8000^{\circ}\text{K}$										
		1	2	3	4	5	6	7	8	9	10	11
P	q	1	2	3	4	5	6	7	8	9	10	11
1	-	1.3(-14)	1.8(-16)	2.6(-17)	8.1(-18)	3.6(-8)	1.9(-18)	1.1(-18)	7.5(-19)	5.2(-19)	3.8(-19)	
2	8.8(-9)	-	4.4(-8)	3.6(-9)	9.3(-10)	3.7(-10)	1.9(-10)	1.1(-10)	7.0(-11)	4.8(-11)	3.4(-11)	
3	8.1(-10)	3.0(-7)	-	1.6(-6)	2.1(-7)	6.5(-8)	2.9(-8)	1.6(-8)	9.6(-9)	6.3(-9)	4.4(-9)	
4	1.7(-10)	3.7(-8)	2.4(-6)	-	1.0(-5)	1.5(-6)	5.0(-7)	2.4(-7)	1.3(-7)	8.2(-8)	5.5(-8)	
5	5.4(-11)	9.3(-9)	3.0(-7)	1.0(-5)	-	3.5(-5)	5.4(-6)	1.8(-6)	8.9(-7)	5.0(-7)	3.2(-7)	
6	2.1(-11)	3.3(-9)	8.4(-8)	1.3(-6)	3.1(-5)	-	8.9(-5)	1.4(-5)	4.8(-6)	2.3(-6)	1.3(-6)	
7	9.6(-12)	1.4(-9)	3.2(-8)	3.8(-7)	4.0(-6)	7.6(-5)	-	1.9(-4)	2.9(-5)	1.0(-5)	4.9(-6)	
8	4.9(-12)	7.0(-10)	1.4(-8)	1.5(-7)	1.2(-6)	9.9(-6)	1.6(-4)	-	3.6(-4)	5.4(-5)	1.9(-5)	
9	2.7(-12)	3.8(-10)	7.5(-9)	7.0(-8)	4.7(-7)	2.9(-6)	2.1(-5)	3.0(-4)	-	6.1(-4)	9.3(-5)	
10	1.6(-12)	2.2(-10)	4.2(-9)	3.7(-8)	2.3(-7)	1.2(-6)	6.1(-6)	3.9(-5)	5.2(-4)	-	9.9(-4)	

The brackets give the powers of 10 by which the entries must be multiplied.

TABLE A-10 (continued)

		$T_e = 16000^\circ K$									
		$T_e = 32000^\circ K$									
		$T_e = 64000^\circ K$									
P		9	1	2	3	4	5	6	7	8	9
1	-	2.2(-11)	1.1(-12)	2.7(-13)	1.0(-13)	5.2(-14)	3.0(-14)	1.9(-14)	1.3(-14)	9.1(-15)	6.7(-15)
2	8.9(-9)	-	1.8(-7)	2.3(-8)	7.4(-9)	3.3(-9)	1.8(-9)	1.1(-9)	7.3(-10)	5.1(-10)	3.7(-10)
3	8.2(-10)	3.2(-7)	-	2.7(-6)	4.2(-7)	1.5(-7)	7.0(-8)	3.9(-8)	2.5(-8)	1.7(-8)	1.2(-8)
4	1.7(-10)	3.7(-8)	2.5(-6)	-	1.3(-5)	2.1(-6)	7.4(-7)	3.6(-7)	2.1(-7)	1.3(-7)	8.9(-8)
5	5.4(-11)	9.4(-9)	3.1(-7)	1.0(-5)	-	3.8(-5)	6.2(-6)	2.2(-6)	1.1(-6)	6.3(-7)	4.0(-7)
6	2.1(-11)	3.3(-9)	8.3(-9)	1.3(-6)	3.0(-5)	-	9.0(-5)	1.4(-5)	5.1(-6)	2.5(-6)	1.4(-6)
7	9.7(-12)	1.4(-9)	3.1(-8)	3.6(-7)	3.8(-6)	7.1(-5)	-	1.8(-4)	2.8(-5)	1.0(-5)	4.9(-6)
8	4.9(-12)	7.0(-10)	1.4(-8)	1.4(-7)	1.1(-6)	9.1(-6)	1.4(-4)	-	3.3(-4)	5.1(-5)	1.8(-5)
9	2.7(-12)	3.8(-10)	7.3(-9)	6.7(-8)	4.4(-7)	2.6(-6)	1.9(-5)	2.7(-4)	-	5.4(-4)	8.3(-5)
10	1.6(-12)	2.2(-10)	4.1(-9)	3.5(-8)	2.1(-7)	1.1(-6)	5.5(-6)	3.4(-5)	4.5(-4)	-	8.6(-4)
		9	1	2	3	4	5	6	7	8	9
1	-	9.1(-10)	9.3(-11)	2.7(-11)	1.2(-11)	6.3(-12)	3.8(-12)	2.5(-12)	1.7(-12)	1.2(-12)	9.0(-13)
2	9.1(-9)	-	3.7(-7)	5.9(-8)	2.1(-8)	9.8(-9)	5.5(-9)	3.4(-9)	2.3(-9)	1.6(-9)	1.2(-9)
3	8.3(-10)	3.3(-7)	-	3.4(-6)	5.8(-7)	2.1(-7)	1.0(-7)	5.9(-8)	3.8(-8)	2.5(-8)	1.8(-8)
4	1.7(-10)	3.7(-8)	2.5(-6)	-	1.4(-5)	2.3(-6)	8.3(-7)	4.1(-7)	2.4(-7)	1.5(-7)	1.0(-7)
5	5.5(-11)	9.3(-9)	3.0(-7)	9.7(-6)	-	3.7(-5)	6.1(-6)	2.2(-6)	1.1(-6)	6.4(-7)	4.1(-7)
6	2.1(-11)	3.3(-9)	7.9(-8)	1.2(-6)	2.7(-5)	-	8.2(-5)	1.3(-5)	4.8(-6)	2.3(-6)	1.4(-6)
7	9.7(-12)	1.4(-9)	3.0(-8)	3.3(-7)	3.4(-6)	6.2(-5)	-	1.6(-4)	2.5(-5)	8.9(-6)	4.4(-6)
8	4.9(-12)	6.8(-10)	1.3(-8)	7.8(-7)	7.9(-6)	1.2(-4)	-	2.8(-4)	4.3(-5)	1.5(-5)	
9	2.7(-12)	3.7(-10)	6.8(-9)	6.1(-8)	3.9(-7)	2.3(-6)	1.6(-5)	2.2(-4)	-	4.5(-4)	6.9(-5)
10	1.6(-12)	2.1(-10)	3.8(-9)	3.2(-8)	1.9(-7)	9.3(-7)	4.6(-6)	2.8(-5)	3.7(-4)	-	6.9(-4)

The brackets give the powers of 10 by which the entries must be multiplied.

TABLE A-10 (continued)

$T_e = 64000^\circ\text{K}$		P										
		1	2	3	4	5	6	7	8	9	10	11
1	-	5.8(-9)	8.3(-10)	2.8(-10)	1.3(-10)	6.9(-11)	4.2(-11)	2.8(-11)	1.9(-11)	1.4(-11)	1.0(-11)	
2	9.3(-9)	-	5.2(-7)	9.0(-8)	3.3(-8)	1.6(-8)	9.1(-9)	5.7(-9)	3.9(-9)	2.7(-9)	2.0(-9)	
3	8.3(-10)	3.2(-7)	-	3.6(-6)	6.3(-7)	2.3(-7)	1.2(-7)	6.7(-8)	4.3(-8)	2.9(-8)	2.1(-8)	
4	1.7(-10)	3.5(-8)	2.3(-6)	-	1.3(-5)	2.2(-6)	8.0(-7)	4.0(-7)	2.3(-7)	1.5(-7)	1.0(-7)	
5	5.4(-11)	8.8(-9)	2.7(-7)	8.6(-6)	-	3.2(-5)	5.4(-6)	2.0(-6)	9.8(-7)	5.7(-7)	3.7(-7)	
6	2.1(-11)	3.1(-9)	7.2(-8)	1.0(-6)	2.3(-5)	-	6.9(-5)	1.1(-5)	4.1(-6)	2.0(-6)	1.2(-6)	
7	9.6(-12)	1.3(-9)	2.7(-8)	2.9(-7)	2.9(-6)	5.1(-5)	-	1.3(-4)	2.0(-5)	7.3(-6)	3.6(-6)	
8	4.9(-12)	6.4(-10)	1.2(-8)	1.1(-7)	8.2(-7)	6.5(-6)	9.9(-5)	-	2.2(-4)	3.4(-5)	1.2(-5)	
9	2.7(-12)	3.4(-10)	6.1(-9)	5.2(-8)	3.3(-7)	1.9(-6)	1.3(-5)	1.7(-4)	-	3.5(-4)	5.4(-5)	
10	1.6(-12)	2.0(-10)	3.4(-9)	2.7(-8)	1.5(-7)	7.6(-7)	3.7(-6)	2.2(-5)	2.9(-4)	-	5.3(-4)	

The brackets give the powers of 10 by which the entries must be multiplied.

For non-hydrogenic systems having known energy levels ϵ_p , the more general expressions of (A-52) and (A-53) must be used for the calculation of collision probabilities.

4.4 Electron Collision Induced Bound-Free Transitions

Let $q(p, \epsilon) d\epsilon$ be the cross section for the formation of electrons with energy in the range $\epsilon, \epsilon + d\epsilon$ by collision of an electron having energy E with an atom in the p state. The total ionization cross section is

$$Q_E(p) = \frac{1}{2} \int_0^{E-I_p} q_E(p, \epsilon) d\epsilon \quad (A-60)$$

and the probability of ionization by collision is

$$D(p) = \left(\frac{8}{\pi m} \right)^{1/2} (kT_e)^{-3/2} \int_0^{\infty} q_E(p) \epsilon \exp(-E/kT_e) \quad (A-61)$$

The rate of depopulation of the (p) state due to electron impact ionization is

$$n(p) n_e D(p) \quad (A-62)$$

The inverse process is three-body recombination:



The efficiency of the three-body process may be written in the form

$$F(p) = \left(\frac{8}{\pi m} \right) (kT_e)^{-3} \int_0^{\infty} \int_0^{\infty} \epsilon_1 \epsilon_2 \exp(-\epsilon_1/kT_e) \exp(-\epsilon_2/kT_e) \times \gamma(p|\epsilon_1, \epsilon_2) d\epsilon_1 d\epsilon_2 \quad (A-64)$$

where $\gamma(p|\epsilon_1, \epsilon_2)$ is the probability that an atom is found in the (p) state as a result of the collision with a positive ion and two electrons with energies ϵ_1 and ϵ_2 respectively. The probability is related to the inverse process of electron impact ionization by detailed balancing. Thus

$$(I_p + \epsilon_1 + \epsilon_2) q_E(p|\epsilon_1) = \frac{16\pi m \omega_1}{h^3 \omega_p} \epsilon_1 \epsilon_2 \gamma(p|\epsilon_1, \epsilon_2) \quad (A-65)$$

Where ω_1 is the statistical weight of the continuum electron and

$$E = I_p + \epsilon_1 + \epsilon_2 . \quad (A-66)$$

The rate of population of level (p) by the three-body recombination process (Equation A-63) is then

$$n_e^2 n(X^+) F(p) \quad (A-67)$$

Alternatively, the probability of three-body recombination $F(p)$ may be obtained by a simpler method noted by Ivanov-Kholodnyi, et al (A-13). They remark that in thermodynamic equilibrium, the number of particles leaving a given quantum level via any specific process is equal to the number of particles entering this state via the inverse process. It follows that

$$F(p) = \varphi(p) D(p) \quad (A-68)$$

where

$$\varphi(p) = p^2 \left(\frac{2\pi m k T_e}{h^2} \right)^{-3/2} \exp(-I_p/kT_e) \quad (A-69)$$

As in the case of excitation, the cross sections decrease too rapidly as the energy of impact increases. Since ionization and its inverse are the controlling processes, the error may be serious and we have therefore given some attention to the problem of how we may obtain improved accuracy, whilst still retaining the universal applicability and the simplicity of the Gryzinski method. A new universal method that has resulted is described below.

Again for reasons similar to those mentioned above for bound-bound collision probabilities, the most accurate method for computing electron impact ionization probabilities, which is of universal applicability is that of Gryzinski^(A-23). Giovanelli^(A-10) and Elwert^(A-12) used the classical Thomson formula which can be expected to give somewhat less accurate results than that of Gryzinski. Ivanov-Kholodnyi et al^(A-13) employed approximate expressions similar to those for the collisional excitation cross-sections.

The classical Thomson cross-section (cf. Thomson^(A-24) or Fowler^(A-25)) for the ionization of an atom having n_0 valence electrons by an electron with energy ϵ , with the corresponding ejection of an electron from a p-state into an energy interval ζ , $\zeta + d\zeta$ is

$$Q_\epsilon(p, \zeta) d\zeta = \frac{4 n_0 \pi a_0^2}{\epsilon(\zeta + \epsilon_p)^2} d\zeta \quad (A-70)$$

The Thomson total ionization cross-section is then

$$Q_\epsilon(p) = \frac{4 n_0 \pi a_0^2}{\epsilon} \int_0^{\epsilon - \epsilon_p} \frac{d\zeta}{(\zeta + \epsilon_p)^2}$$

$$= 4 \pi a_0^2 n_0 \frac{(\epsilon - \epsilon_p)}{\epsilon_p \epsilon^2} \quad (A-71)$$

a_0 is the radius of the first Bohr orbit in hydrogen.

As pointed out in the previous section, the Gryzinski formulas represent an improvement over the Thomson derivation in that account is taken of the motion of the bound atomic electrons. According to Gryzinski the total ionisation cross-section for an electron-electron collision in which the impacting electron suffers an energy loss ΔE greater than the threshold ionization energy ϵ_p is given by

$$Q(\epsilon_p) = \int_{\epsilon_p}^{\Delta E_{\max}} \sigma(\Delta E) d(\Delta E) \quad (A-72)$$

where ΔE_{\max} is the maximum permissible transfer of energy consistent with conservation of momentum and energy, and $\sigma(\Delta E)$ is the differential cross-section described by Equation (A-52). (The expression for $Q(\epsilon)$ given in (A-54) was obtained from the integration indicated by (A-72)). Thus the cross-section for ionization from the p level is just (A-54). The ionization transition probability for a Maxwellian electron energy distribution is given by

$$D(p|T_e) = \left(\frac{3}{\pi m}\right)^{1/2} \frac{1}{(kT_e)^{3/2}} \int_0^{\infty} Q(\epsilon_p) \epsilon e^{-\epsilon/kT_e} d\epsilon \quad (A-73)$$

Making the substitutions $x = \epsilon/\epsilon_p$ we find from (A-54) and (A-73) that

$$D(p|T_e) = \frac{5.45}{T_e^{3/2}} \cdot \begin{cases} \frac{4\sqrt{2}}{3} \int_1^{\infty} \left(\frac{x-1}{x+1}\right)^{3/2} \exp\left\{-\frac{1.5789 \times 10^5 \epsilon_p x}{T_e}\right\} dx & \left(\frac{cm^3}{sec}\right) x < 2 \\ \left(\frac{1}{3}\right)^{1/2} \frac{(5x-6)x^{1/2}}{(x+1)^{3/2}} \exp\left\{-\frac{1.5789 \times 10^5 \epsilon_p x}{T_e}\right\} dx & \left(cm^3/sec\right) x > 2 \end{cases} \quad (A-74)$$

In the case of hydrogen, $\epsilon_p = 1/p^2$ so that

$$D(p|T_e) = \frac{5.45}{T_e^{3/2}} \begin{cases} \frac{4\sqrt{2}}{3} \int_1^{\infty} \left(\frac{x-1}{x+1}\right)^{3/2} \exp\left\{\frac{-1.5789 \times 10^5}{p^2 T_e} x\right\} dx & x < 2 \\ \frac{1}{3} \int_1^{\infty} \frac{(5x-6)x^{1/2}}{(x+1)^{3/2}} \exp\left\{\frac{-1.5789 \times 10^5}{p^2 T_e} x\right\} dx & x > 2 \end{cases} \quad (A-75)$$

Values of $D(p|T_e)$ in hydrogen (provided by Bates) are given in Table A-11 for p less than or equal to 10. For the more general case, Equation (A-74) must be used to compute $D(nl|T_e)$.

As in the case of excitation, the cross-sections decrease too rapidly as the energy of impact increases. Since ionization and its inverse are the controlling processes at the higher energy levels, the error may be serious and we have therefore given some attention to the problem of how to obtain improved accuracy, whilst still retaining the universal applicability and the simplicity of the Gryzinski method.

Rewriting Equation (A-71) for the Thomson ionization cross-section in the form

$$\frac{I^2 Q_i(\epsilon)}{n_0} = 4\pi a_0^2 \frac{I}{\epsilon} \left(1 - \frac{I}{\epsilon}\right) \quad (A-76)$$

and introducing the dimensionless parameter $\lambda = \epsilon/I$

TABLE A-11

		COLLISIONAL IONIZATION COEFFICIENTS FOR HYDROGEN D(Π_e) IN cm^3/sec								
		250	500	1000	2000	4000	8000	16000	32000	64000
		P								
1	6.3(-285)	1.7(-147)	1.3(-78)	5.1(-44)	1.4(-26)	9.6(-18)	3.4(-13)	8.2(-11)	1.5(-9)	
2	1.0(-77)	3.9(-43)	1.1(-25)	7.7(-17)	2.7(-12)	6.6(-10)	1.2(-8)	5.9(-8)	1.3(-7)	
3	9.6(-39)	3.2(-23)	2.6(-15)	3.1(-11)	4.2(-9)	5.8(-8)	2.4(-7)	4.9(-7)	6.7(-7)	
4	8.6(-25)	6.1(-16)	2.2(-11)	5.3(-9)	9.8(-8)	4.7(-7)	1.1(-6)	1.5(-6)	1.7(-6)	
5	3.8(-18)	2.2(-12)	2.1(-9)	8.3(-8)	5.7(-7)	1.6(-6)	2.7(-6)	3.3(-6)	3.3(-6)	
6	2.1(-14)	2.4(-10)	3.3(-8)	4.6(-7)	1.9(-6)	3.9(-6)	5.4(-6)	5.8(-6)	5.4(-6)	
7	4.5(-12)	5.1(-9)	2.1(-7)	1.5(-6)	4.4(-6)	7.4(-6)	9.0(-6)	9.1(-6)	8.1(-6)	
8	1.7(-10)	4.2(-8)	7.8(-7)	3.7(-6)	8.5(-6)	1.2(-5)	1.4(-5)	1.3(-5)	1.1(-5)	
9	2.4(-9)	2.0(-7)	2.1(-6)	7.5(-6)	1.4(-5)	1.8(-5)	2.0(-5)	1.8(-5)	1.5(-5)	
10	1.7(-8)	6.6(-7)	4.7(-6)	1.3(-5)	2.2(-5)	2.6(-5)	2.3(-5)	1.9(-5)		

The brackets give the powers of 10 by which the entries must be multiplied.

(A-47) becomes

$$\frac{I^2 Q_i(\lambda I)}{n_0} = 4\pi a_0^2 \frac{1}{\lambda} \left(1 - \frac{1}{\lambda}\right) \quad (A-77)$$

The right-hand side of (A-77) is a universal function of λ , independent of the particular ionizing process.

It is known from the asymptotic form of the Born approximation (cf. Mott and Massey (A-13)) that for large values of λ , Q_i behaves asymptotically according to

$$Q_i \sim \lambda^{-1} \ln \lambda \quad (A-78)$$

so that (A-77) is incorrect in the limit of high impact energies.

The modification of (A-71) by Gryzinski (A-23) also has this defect.

We shall attempt to improve (A-77) by introducing a correcting factor $f(\lambda)$ such that

$$\begin{aligned} \frac{I^2 Q_i(\lambda I)}{n_0} &= 4\pi a_0^2 \frac{1}{\lambda} \left(1 - \frac{1}{\lambda}\right) f(\lambda) \\ &= 4\pi a_0^2 g(\lambda) \end{aligned} \quad (A-79)$$

and determine $f(\lambda)$ by appeal to experimental data.

In figure (A-2), all the available experimental data (A-26 thru A-33) on the electron impact single ionization of atoms has been used to determine $I^2 Q_i/n_0$ as a function of λ , adopting for n_0 the number of electrons in the valence shell. If $f(\lambda)$ exists such that (A-79) is true, this procedure would produce a single curve. Instead,

there results distinct curves which are similar in shape but have an appreciable spread in magnitude of the cross-sections. This spread represents the possible error that would be a consequence of the use of the mean of the curves of Figure (A-2) as a universal function.

We may reduce this factor by taking partial account of the electron structure of the atomic systems, it being an oversimplification to adopt for n simply the number of valence electrons n_0 . The significant quantity is actually the equivalent number of dispersion electrons for transitions into the continuum.

To determine n , we may proceed in two alternative ways. We may choose n to ensure all the curves have the same magnitude at large energies or we may observe from (A-71) that the maximum value of Q_i is given by

$$Q_i^{\max} = \frac{n_0 \pi a_0^2}{I^2} \quad (A-80)$$

and determine n from

$$n = \frac{Q_i^{\max} I^2}{\pi a_0^2} \quad (A-81)$$

The latter procedure is the simpler and we adopt it. It leads to the curves shown in Figure (A-3), all of the normalized experimental data for ionization of neutral atoms lies within the shaded area. No curve now departs from the mean of all the curves by a factor of more than about 10% (cf shaded area of Figure A-3) and we shall select the mean as a universal curve. The normalized curve for ionization of

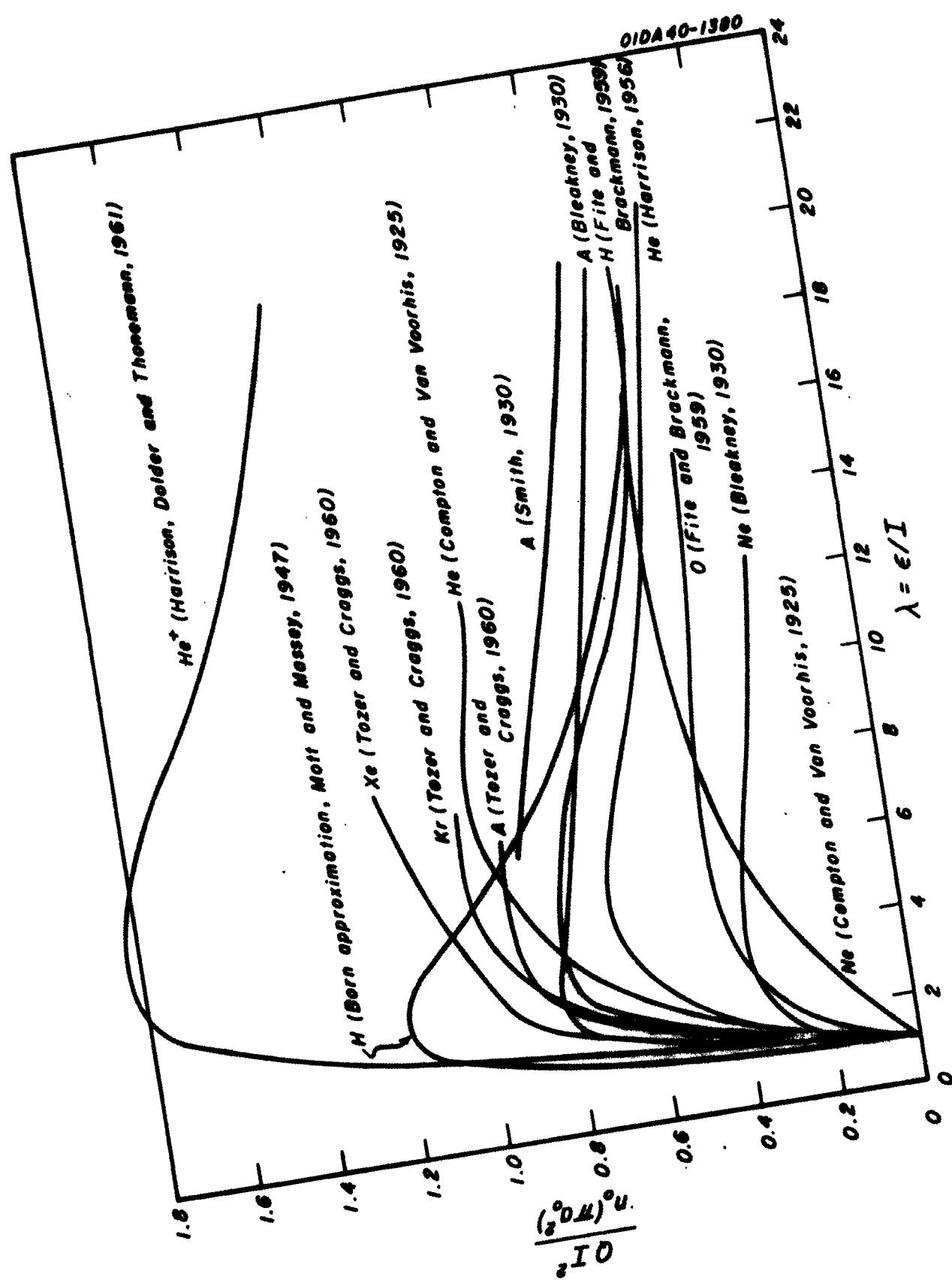


Figure A-2. Summary of Experimental Electron Collision Ionization Cross Sections

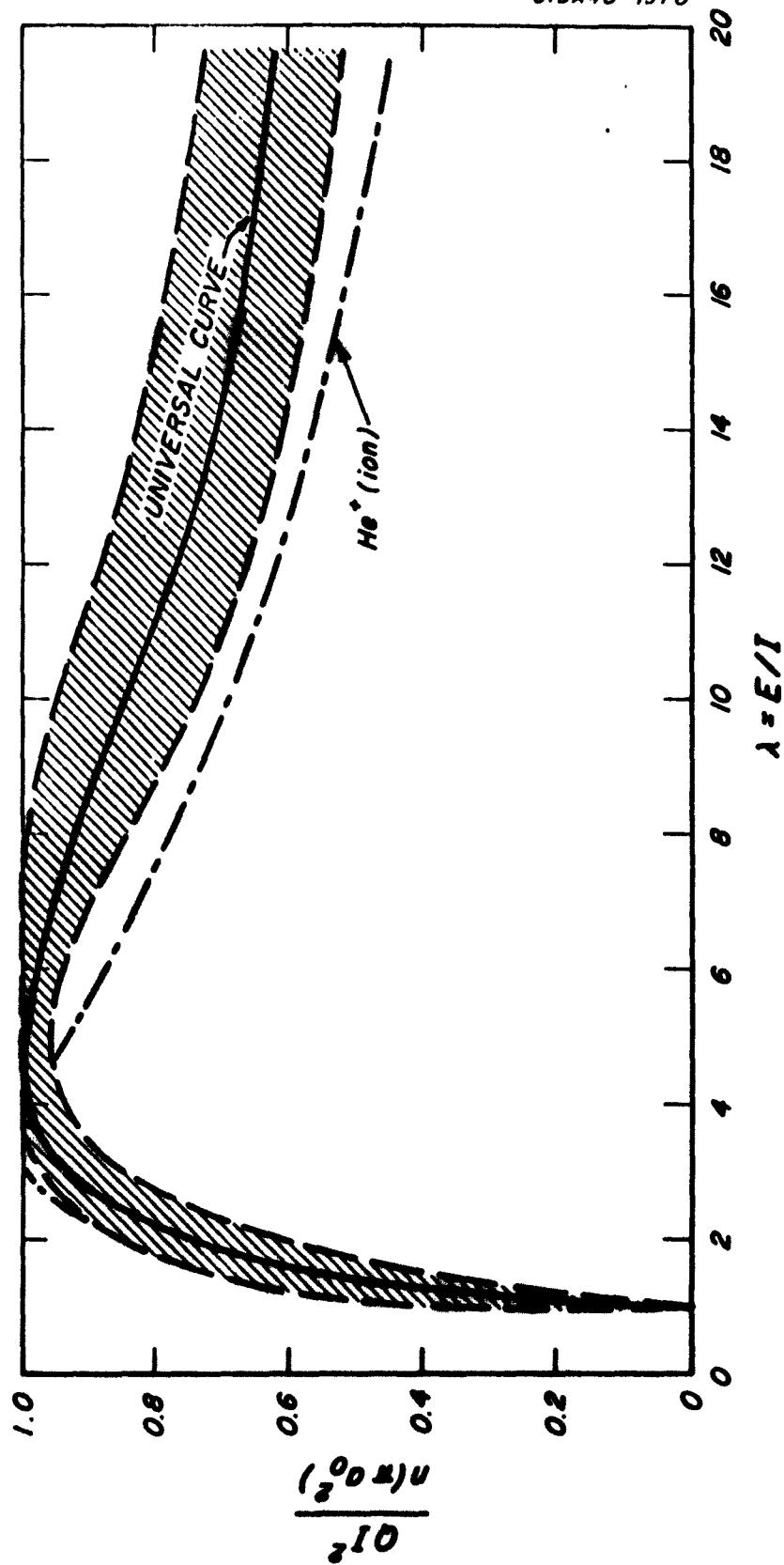


Figure A-3. Universal Curve for Electron Impact Ionization Cross Sections

of He^+ ion falls just outside of this area and is also shown in Figure A-3.

The corresponding values of n are given in Table (A-12a). We see that there is a pattern to n which allows us to predict it with some reliability at least for the lighter elements. Thus, since n appears to be an increasing function of atomic number, we can assign integer values of n to appropriate ranges of the atomic number as shown in Table (A-12b).

From the universal curve of Figure (A-3), we can proceed to the determination of a universal ionization probability curve as a function of electron temperature T_e . Thus from Equation (A-58) we find

$$D(T_e) = \left(\frac{8}{\pi m}\right)^{1/2} (kT_e)^{-3/2} \int_0^\infty Q_i(\lambda, I) \lambda e^{-\lambda I/kT_e} I^2 d\lambda \quad (\text{A-82})$$

Using Equation (A-77)

$$D(T_e) = \left(\frac{8}{\pi m}\right)^{1/2} (kT_e)^{-3/2} 4\pi n a_0^2 \int_1^\infty \lambda g(\lambda) e^{-\lambda/kT'_e} d\lambda \quad (\text{A-83})$$

where $T'_e = T_e/I$ is the electron temperature measured in units of the ionization potential. Finally

$$D(T_e) T_e^{3/2} = \left(\frac{8}{\pi m k}\right)^{1/2} 4\pi n a_0^2 \int_1^\infty \lambda g(\lambda) e^{-\lambda/kT'_e} d\lambda \quad (\text{A-84})$$

The right hand side of which is a function of the electron temperature T'_e only and may be computed once for all atomic systems for any given value of T'_e , using the universal curve $g(\lambda)$ given in Figure (A-3).

TABLE A-12a
EQUIVALENT NUMBER OF DISPERSION ELECTRONS,
n DETERMINED BY EQUATION (A-81)

Element	H	He	O	Ne	A	Kr	Xe	Hg
n_o	1	2	4	6	6	6	6	2
n	0.8	1.34	1.75	2.24	4.20	6.05	7.14	3.74

TABLE A-12b
ESTIMATED VALUE OF n

	n
H - Be	1
B - Ne	2
Na - A	4
K - Kr	6
Cs - Xe	7

The function $\frac{DT}{n} \frac{e^{3/2}}{e}$ is shown as a function of T' in Figure (A-4).

The ionization probability for any element for any temperature may be read off the graph, the appropriate abscissa being obtained by dividing T_e by the ionization potential I .

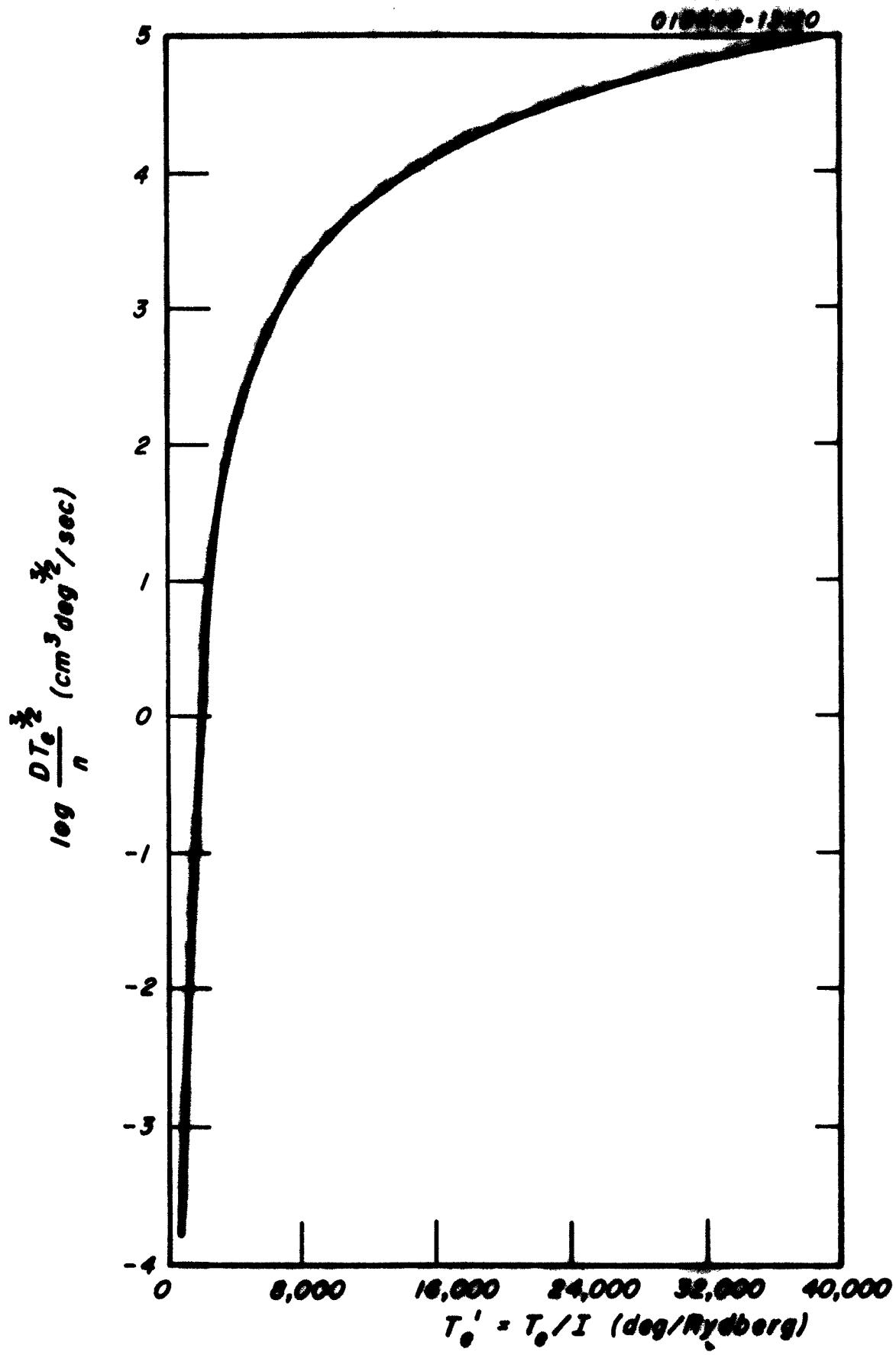


Figure A-4. Universal Ionization Probability Curve

A.5 Heavy Particle Collisions

Consider now transitions produced by collisions with heavy particles which we label Y_i . Let $Q_\epsilon^i(p, r)$ be the cross section for the excitation to the r^{th} state by the impact of a heavy particle Y_i with an atom X in the p^{th} state, the energy of relative motion being ϵ . The rate of depopulation of the p^{th} state by heavy particle impact is

$$n(p) \sum_i n(Y_i) \sum_{r>p} P_i(p, r) \quad (\text{A-85})$$

where the collision probability $P_i(p, r)$ is obtained by multiplying the cross section by the relative velocity of the collision and integrating over ion velocity distribution $f(v)$ to give

$$P_i(p, r) = \int v Q_r^i(p, r) f(v) dv \quad (\text{A-86})$$

If $f(v)$ is the Maxwellian velocity distribution corresponding to temperature T ,

$$P_i(p, r) = \frac{2}{\pi \mu_i}^{\frac{1}{2}} (kT)^{-3/2} \int_{I_r - I_p}^{\infty} Q_r^i(p, r) \epsilon \exp(-\epsilon/kT) d\epsilon \quad (\text{A-87})$$

where μ_i is the reduced mass.

The probability of de-excitation to a lower level is similarly given by

$$n(p) \sum_i n(Y_i) \sum_{q<p} P_i(p, q) \quad (\text{A-88})$$

The rates of population are

$$\sum_i n(Y_i^+) \sum_{q < p} n(q) P_i(q, p) \quad (A-89)$$

and

$$\sum_i n(Y_i^+) \sum_{r > p} n(r) P_i(r, p) \quad (A-90)$$

The ionization and recombination involving collision with ions may be formulated in a manner similar to that for electron collisions. The rate of depopulation by ion impact induced ionization may be written

$$n(p) \left\{ n(X^+) Q(p) + \sum_j n(Y_j^+) Q_j(p) \right\} \quad (A-91)$$

$$Q(p) = \frac{1}{(\pi M_X)^{1/2}} (kT)^{-3/2} \int_0^\infty Q_E(p) \exp(-E/2kT) dE \quad (A-92)$$

$Q_E(p)$ is the total ionization cross section of the state (p) by ions of energy E.

The rate of population by three-body recombination



may be written

$$n(X^+) n(Y_i^+) R(p) \quad (A-94)$$

where $R(p)$ is an expression exactly similar to Equation (A-64)

Since for allowed transitions the cross sections for the impact of an electron and a singly charged positive ion of the same velocity are of much the same size, excitation and ionization by ion impact is usually very inefficient compared to electron impact. For example, three-body recombination



will be negligible compared to



Exceptions may occur when the energy defect of the process is small as in



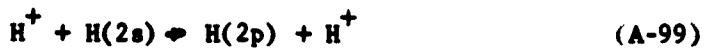
and for transitions between pairs of highly excited states. The effects of ion impacts is to strengthen the argument that a Boltzmann equilibrium prevails for the excited states. The position regarding charge transfer reactions is analogous, charge transfer being rapid at low velocities only when the energy defect is low.

We merely wish to provide a few numbers in order to show quantitatively that, apart from re-distributing processes, (and transitions between pairs of highly excited states), electron collisions are more efficient than heavy particle collisions.

Seaton^(A-34) has calculated the rate coefficient for the re-distribution process

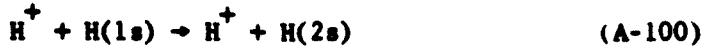


at 10,000°K, and he obtains the very large value of about $5 \times 10^{-4} \text{ cm}^3 \text{ sec}^{-1}$. Re-distribution may also occur by charge transfer



but Boyd and Dalgarno^(A-35) have shown that (A-99) is much less rapid than (A-98).

Excitation and ionization proceed much more slowly and may be neglected. Thus, the maximum values of the cross sections for the direct processes



are respectively about $5 \times 10^{-17} \text{ cm}^2$ at about 20 kev impact energy, (Bates^(A-36)) and $1 \times 10^{-16} \text{ cm}^2$ at about 30 kev (Bates^(A-37)) and the cross sections are decreasing rapidly with decreasing energy.

Similarly, it may be seen from the calculations of Bates and Dalgarno^(A-38,A-39) that excitation accompanying charge transfer such as

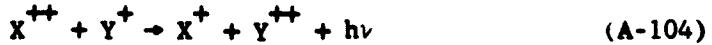


is extremely inefficient for temperatures below several kev.

Thus, for a hydrogen plasma or other singly ionized plasma of a single component, processes due to ion impact may be ignored. When more than one component exists in a plasma, however, it may be necessary to consider heavy particle processes, for charge transfer processes are unique in coupling together the two components. This fact may be seen from Equation (A-106), by noting that if the heavy body coefficients P_i , Q_i , and R_i are set equal to zero, all the terms containing $n(Y_i)$, the number density of other ions vanish. Account must be taken not only of ordinary charge transfer

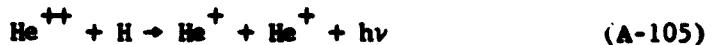


but also of radiative charge transfer



which may be more rapid than the previous reaction.

An investigation of the possible rates of these charge transfer reactions, one of the participants of which is an ionic system in its ground state, is necessary, and as an example of the latter process



may be treated with high accuracy.

Special features also arise in the case of a single component plasma in which the component may exist in more than one state of ionization.

A.6 The Basic Equations

The increase in population per second of a particular level (p) is given by the difference between the rates of population and depopulation that we have written in the earlier sections. Thus

$$\begin{aligned}
 \frac{dn(p)}{dt} = & \left\{ \left[\sum_{q < p} A(p, q) \{1 + X(p, q)\} + \frac{1}{\omega_p} \sum_r \omega_r X(p, r) A(r, p) \right] \right. \\
 & + n_e \left[\sum_r C(p, r) + \sum_q C(p, q) + D(p) \right] \\
 & + \sum_i n(Y_i) \left[\sum_r P_i(p, r) + \sum_q P_i(p, q) + Q_i(p) \right] \\
 & \left. + \beta(p) \right\} n(p) \\
 = & - \sum_r \left\{ A(r, p) [1 + X(r, p)] + n_e C(r, p) + \sum_i n(Y_i) P_i(r, p) \right\} n(r) \\
 & + \sum_q \left\{ \frac{\omega_p}{\omega_q} X(q, p) A(p, q) + n_e C(q, p) + \sum_i n(Y_i) P_i(q, p) \right\} n(q) \\
 & + \alpha(p) n_e X(n^+) + n_e^2 X^+ y_f(p) \\
 & + n_e \sum_i n_i(Y_i^+) n(X^+) R_i(p) \tag{A-106}
 \end{aligned}$$

We arrive at a set of coupled, differential equations of the form

$$\frac{dn(p)}{dt} + a_{pp} n(p) = \sum_{j \neq p} a_{pj} n_j + b_p \tag{A-107}$$

where the a 's and b 's can be identified by comparison with the preceding equation.

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APPENDIX B
A. Naqvi

ATOMIC TRANSITION PROBABILITIES

B.1 INTRODUCTION

Consider two energy levels, 1 and 2, of any atom, and let their energies, E_1 and E_2 , be such that $E_2 > E_1$. Transitions from 2 to 1 result in emission, and the reverse transitions, from 1 to 2, are, among other processes, caused by the absorption of radiation, of frequency ν_{21} given by

$$E_2 - E_1 = h \nu_{21} \quad (B-1)$$

The amount of energy (in $\text{erg cm}^{-3} \text{ sec}^{-1}$) emitted in a spectral line is given by

$$E_{21} = n_2 [A(2,1) + B(2,1) I_{21}] \quad (B-2)$$

where n_2 is the number of atoms per cm^3 in level 2. $A(2,1)$ and $B(2,1)$ are, respectively, the probabilities (in sec^{-1}) of spontaneous transitions and the transitions stimulated by the presence of an external radiation field. I_{21} is the intensity of this external radiation field at the frequency ν_{21} .

Similarly the amount of energy (in $\text{ergs cm}^{-3} \text{ sec}^{-1}$) absorbed in a spectral line is given by

$$E_{12} = n_1 B(1,2) I_{21} h \nu_{21} \quad (B-3)$$

where $B(1,2)$ is the probability of the upward transition, from level 1 to level 2, with the absorption of radiation of frequency ν_{21} .

The three transition probabilities are related to each other by the following relations due to Einstein.

$$B(2,1) = \frac{g_1}{g_2} B(1,2) \quad (B-4)$$

$$A(2,1) = \frac{g_1}{g_2} \frac{2 h \nu_{12}^3}{c^2} B(1,2) \quad (B-5)$$

where g_1 and g_2 are the statistical weights of the two levels. It is therefore sufficient to determine one of the three transition probabilities, usually $A(2,1)$.

The theory for calculating atomic transition probabilities for electric dipole radiation is well known (Condon and Shortley^(B-1), Slater^(B-2)). Several reviews have been written in recent years also (Garstang^(B-3), Maqvi^(B-4)). The probability $A(2,1)$ of a spontaneous radiative transition is given by

$$A(2,1) = \frac{64\pi^4}{3\hbar g_2} \frac{1}{\lambda^5} S(2,1) \quad (B-6)$$

where g_2 is the statistical weight of level 2, λ is the wavelength of the spectral line emitted, $S(2,1)$ is known as the line strength and for LS coupling can be written as

$$S(2,1) = S(1,2) = J(L)J(M) \sigma^2 \quad (B-7)$$

where $J(L)$ and $J(M)$ are factors which arise as a result of integration over the angular part of the wave function. $J(L)$ is known as the relative strength of a line within the multiplet to which it belongs and $J(M)$ is known as the relative multiplet strength. Both of these quantities can be calculated in a closed form for any given line and any given multiplet. $J(L)$ has been tabulated by White and Eliason^(B-5) and by Russell^(B-6). $J(M)$ has been tabulated by Goldberg^(B-7 and B-8). These tables have also been reproduced by Allen^(B-9). Recently Rohrlich^(B-10) has derived general expressions, based on Racah's method, from which multiplet strengths for transitions not covered by Goldberg can be obtained.

The electric-dipole transition integral σ^2 is given by

$$\sigma^2(n_1 l_1, n_2 l_2) = \frac{1}{4l_2^2 - 1} \left[\int_0^{\infty} P(n_1 l_1; r) P(n_2 l_2; r) dr \right]^2 \quad (B-8)$$

where the P's are r times the radial wave functions, and l_2 is the greater of the two azimuthal quantum numbers l_1 and l_2 . The calculation of the

absolute transition probabilities therefore depends upon the calculation of the transition integral σ^2 , which in turn depends upon an appropriate choice of the radial wave functions.

B.2 THE RADIAL WAVE FUNCTIONS

The radial wave functions, $P(nl;r)$, are the solutions of the radial part of the non-relativistic Schrödinger equation,

$$\left\{ \frac{d^2}{dr^2} + 2 \left[E - V(r) \right] - \frac{l(l+1)}{r^2} \right\} P(nl;r) = 0 \quad (B-9)$$

where E is the eigen value of the Hamiltonian for a given stationary state and $V(r)$ is the central field in which the electron moves. Note that atomic units are used throughout this report.

The importance of a knowledge of the radial wave functions cannot be over emphasized. The radial wave function, in a nutshell, gives us an insight into all other physical properties of the atom. A knowledge of the radial wave functions is required not only in the calculation of the transition probabilities but also photoionization cross sections, elastic scattering cross-sections, collision cross-sections for excitation of atoms, x-ray scattering and numerous molecular and solid state properties, among others.

The most commonly used method is the self-consistent field method, developed by Hartree and extended by Fock to include exchange effects (for a recent review, see Hartree^(B-11)). These are obtained by numerical

solution of a system of simultaneous, inhomogeneous, non-linear, integro differential equations, the so-called Fock equations. Efforts have also been made to include the effects due to configuration mixing and correlation of electrons. (See Hartree^(B-11)), The procedure is very laborious, and has to be performed separately for each configuration of each atom. Since numerical methods are used the results are given in a tabular form, and cannot be used for further analytical calculations. It is, therefore, not possible to develop analytical methods of great generality, but every problem must be solved separately. Thus although the theory was developed in all essential details over 30 years ago, a list of atoms and their configurations for which the self-consistent field radial wave functions are available is pitifully small. In particular it is clear that if one wants to calculate atomic parameters, such as transition probabilities, for a large number of atoms one must develop methods of considerable generality which can, at one time, be applied to a large number of cases.

On account of their obvious usefulness, many attempts have been made to obtain analytic wave functions (for example Zener^(B-12); Eckert^(B-13); Slater^(B-14); Morse, Young and Haurwitz^(B-15); Tubis^(B-16); Morse and Yilmaz^(B-17); Breene^(B-18 and B-19); Roothan, Sachs and Weiss^(B-20)). Some of these were merely attempts to obtain analytical expressions of which the parameters were determined by comparison with the tabular wave functions of the self-consistent field method.

Since the advent of quantum theory, it has been very tempting to use the exact results obtained for hydrogen, for the more complex atoms

also, by the substitution of either an "effective" principal quantum number n^* for n , or a "screened" nuclear charge Z_α ($= Z - s_\alpha$) for the actual nuclear charge Z . Here s_α denotes the screening of an electron α by all the other electrons in the atom. The screening parameters have been determined usually by a semi-empirical method (Pauling^(B-21) ; Pauling and Sherman^(B-22)), although a variational treatment has been applied to some simple cases. The interest in the use of hydrogenic wave functions with a screened nuclear charge has been revived through a method for calculating the screening parameters developed by Layzer^(B-23)

B.3 THE HYDROGENIC WAVE FUNCTIONS

The screened hydrogenic radial wave functions, briefly referred to as the "hydrogenic wave functions", are the solutions of Equation B-9 with $V(r)$ replaced Z_{nl}/r , the Coulomb potential due to a screened nuclear charge Z_{nl} ($= Z - s_{nl}$), where s_{nl} is a screening parameter and Z is the atomic number. They are given by

$$P(nl Z_{nl}; r) = - \left[\frac{(n+l)!}{(2n)(n^*)!} \right]^{\frac{1}{2}} \frac{r^{l+1}}{(2l+1)!}$$

$$\cdot \exp \left[-\frac{Z_{nl}}{n} r \right] \left(\frac{2}{n} Z_{nl} \right) {}_1F_1 \left(-n^*, 2l+2; \frac{2}{n} Z_{nl} r \right) \quad (B-10)$$

where n^* denotes $(n-l-1)$, the number of nodes of the function and ${}_1F_1$ is a confluent hypergeometric function defined below. Because of the way

Z_{ne} occurs in Equation B-10, we shall find it convenient to substitute in the above equation,

$$\gamma_{ne} = \frac{2}{n} Z_{ne} = \frac{2}{n} Z - \frac{2}{n} s_\alpha = \gamma - \pi_\alpha \quad (B-11)$$

where γ equals $2Z/n$ and π_α ($= 2s_\alpha/n$) is a reduced screening parameter.

We now have

$$P(nl \gamma_{ne}; r) = -Q_{ne} \gamma_{ne}^{l+\frac{3}{2}} r^{l+1} \cdot \exp[-\frac{1}{2} \gamma_{ne} r] {}_1F_1(-n^*, 2l+2; \gamma_{ne} r) \quad (B-12)$$

where

$$Q_{ne} = \left[\frac{(n+l)!}{(2n)(n^*)!} \right]^{1/2} \frac{1}{(2l+1)!} \quad (B-13)$$

and

$${}_1F_1(-n^*, 2l+2; \gamma_{ne} r) = \sum_{i=0}^{n^*} {}_i d_{ne} \gamma_{ne}^i r^i \quad (B-14)$$

where

$${}_i d_{ne} = (-1)^i \frac{(n^*)!}{(n^*-i)!} \frac{(2l+1)!}{(2l+1-i)!} \frac{1}{i!} \quad (B-15)$$

It is to be noted that γ_{nl} is different for different nl and that the radial wave functions (Equations B-10 or B-12) for the same n but different l are not strictly orthogonal. It is possible to make corrections due to the lack of orthogonality of the wave functions, but they are not considered in this report.

For subsequent use in calculating the Slater F integrals we write below an expression for the square of the radial wave function (Equations B-12 and B-14).

$$\left[P(nl\gamma_{nl}; r) \right]^2 = Q_{nl} \gamma_{nl}^{2l+3} r^{2l+2} \exp[-\gamma_{nl} r] \\ \cdot \sum_p^{2n^*} d_{np}^p \gamma_{np}^p r^p \quad (B-16)$$

where

$$d_{np}^p = \sum_i^n d_{np}^i d_{nl}^{p-i} \quad (B-17)$$

B.4 RESUME OF LAYER'S SCREENING THEORY

Layzer^(B-23) has shown that the eigen values of energy will possess the correct quadratic and linear Z-dependence if the one-electron radial wave functions satisfy the condition that,

$$P(nl\gamma; r) = P^H(nl\gamma; r) + O(nl\gamma; r) \quad (B-18)$$

where the superscript H denotes a hydrogenic wave function and $O(n\ell \gamma; r)$ denotes a term of order one in γ , and

$$\frac{O(n\ell \gamma; r)}{P(n\ell \gamma; r)} = O(\gamma^{-1}) \quad (B-19)$$

so that, at least, for large γ , $O(n\ell \gamma; r)$ term can be neglected. Note that our notation differs slightly from that used by Layzer.

Neglecting $O(n\ell \gamma; r)$ terms, and applying the variational principle Layzer has shown that the screening parameter π_α , which gives the screening of the electron α by all the other electrons in the atom, is given by

$$\pi_\alpha = \frac{4}{q_\alpha} \frac{\partial V_1}{\partial \gamma_\alpha} \quad (B-20)$$

where V_1 denotes the matrix elements of the Coulomb interaction energy and q_α denotes the number of electron in the subshell α . We can use several different approximations for the Coulomb interaction, for example we may or may not include configuration mixing and we may either consider the average energy of a given configuration or we may add to it the contributions which come from different spectroscopic terms (characterized by quantum numbers S and L), belonging to the same configuration.

In the work reported here, we have not considered configuration mixing, but we consider the energy of individual terms as well as the average energy of the configuration. When required, the screening constants which are dependent on SL can be labelled explicitly as $\pi_{n/SL}$,

whereas those based on the average energy will be labelled as $\pi_{n\ell}$.

The term energies as functions of the screening parameters are given by

$$W(\pi) = -\frac{1}{8} \sum_{\alpha} q_{\alpha} (\gamma - \pi_{\alpha}) \quad (B-21)$$

where the summation is over all the subshells in the atom. This is a very simple formula for calculating the term energies from the screening parameters.

B.5 THE COULOMB INTERACTIONS OF ELECTRONS

The most commonly used approximation for complex atoms (see, for example, Condon and Shortley^(B-1)) is the separable wave function approximation in which each electron is assumed to be in a stationary state in the field of the nucleus and all the other electrons. The wave function of an N -electron atoms is expressed in the form of a determinant, made up of the wave functions of individual electrons, as follows,

$$\Phi = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(a^1) & u_2(a^1) & \dots & u_N(a^1) \\ u_1(a^2) & u_2(a^2) & \dots & u_N(a^2) \\ \dots & \dots & \dots & \dots \\ u_1(a^N) & u_2(a^N) & \dots & u_N(a^N) \end{vmatrix} \quad (B-22)$$

where u is the wave function of the single electron problem, a^i denotes the set of quantum numbers (n^i, l^i, m_s^i, m_l^i) and subscripts of u , from 1 to N , denote the electron to which this wave function belongs. The determinantal form insures the antisymmetry property of the wave functions.

For a many-electron wave function of the above form, Slater^(B-24) has shown that the matrix elements of the mutual Coulomb interactions of the electrons, $1/r_{ij}$, are sums of the matrix elements of the corresponding two electron problem.

Ignoring configuration mixing, the average electrostatic energy of a configuration may be written as

$$V_{av} = \sum_{\alpha < \beta} q_{\alpha\beta} \{ \alpha, \beta \} \quad (B-23)$$

where

$$q_{\alpha\beta} = (1 - \frac{1}{2} \delta_{\alpha\beta}) q_{\alpha} (q_{\beta} - \delta_{\alpha\beta}) \quad (B-24)$$

and the two electron interaction $\{ \alpha, \beta \}$ is given by

$$\begin{aligned} \{ \alpha, \beta \} &= \sum_k^{\alpha < l} f^k(l_{\alpha} l_{\beta}) F^k(\alpha, \beta) \\ &+ \sum_{\substack{l_{\alpha} + l_{\beta} \\ l_{\alpha} - l_{\beta}}}^{\alpha < l} g^k(l_{\alpha} l_{\beta}) G^k(\alpha, \beta) \end{aligned} \quad (B-25)$$

where the prime over the summation sign indicates that k does not assume all integral values, but for F^k all even integral values and for G^k either all even or all odd integral values. $l_{<}$ denotes the lesser of l_{α} and l_{β} .

The coefficients $f^k(l_\alpha l_\beta)$ and $g^k(l_\alpha l_\beta)$ arise from the angular and the spin part of the wave functions. These can be calculated by the well known matrix methods. For details of these calculations the reader is referred to Condon and Shortley^(B-1) and to the more powerful methods, due to Racah^(B-25), based on tensor operators. These coefficients are listed in Tables B-1 and B-2.

F^k and G^k are integrals over the radial part of the wave functions, also known as Slater integrals. They are defined by

$$\begin{aligned}
 R^k(n_\alpha l_\alpha n_\beta l_\beta, n_\gamma l_\gamma n_\delta l_\delta) \\
 = \int_0^\infty \int_0^\infty \frac{r^k}{r_>^{k+1}} P(n_\alpha l_\alpha; r_1) P(n_\beta l_\beta; r_2) \\
 \cdot P(n_\gamma l_\gamma; r_1) P(n_\delta l_\delta; r_2) dr_1 dr_2 \quad (B-26)
 \end{aligned}$$

with

$$F^k(n_\alpha l_\alpha, n_\beta l_\beta) \equiv R^k(n_\alpha l_\alpha n_\beta l_\beta, n_\alpha l_\alpha n_\beta l_\beta) \quad (B-27)$$

and

$$G^k(n_\alpha l_\alpha, n_\beta l_\beta) \equiv R^k(n_\alpha l_\alpha n_\beta l_\beta, n_\beta l_\beta n_\alpha l_\alpha) \quad (B-28)$$

TABLE B-1

COEFFICIENTS OF SLATER INTEGRALS FOR EQUIVALENT ELECTRONS
 (For a tabulated value of ℓ_α all non-vanishing coefficients are listed)

ℓ_α	$f^0(\ell_\alpha \ell_\alpha)$	$f^2(\ell_\alpha \ell_\alpha)$	$f^4(\ell_\alpha \ell_\alpha)$	$f^6(\ell_\alpha \ell_\alpha)$
0	1	0	0	0
1	1	-2/25	0	0
2	1	-2/63	-2/63	0
3	1	-4/195	-2/143	-100/5577

TABLE B-2

COEFFICIENTS OF SLATER INTEGRALS FOR NON-EQUIVALENT ELECTRONS
 (For a tabulated combination $(\ell_\alpha, \ell_\beta)$ all non-vanishing coefficients are listed)

ℓ_α	ℓ_β	f^0	g^0	g^1	g^2	g^3	g^4	g^5	g^6
0	0	1	-1/2	0	0	0	0	0	0
0	1	1	0	-1/6	0	0	0	0	0
0	2	1	0	0	-1/10	0	0	0	0
0	3	1	0	0	0	-1/14	0	0	0
1	1	1	-1/6	0	-1/15	0	0	0	0
1	2	1	0	-1/15	0	-3/70	0	0	0
1	3	1	0	0	-3/70	0	-2/63	0	0
2	2	1	-1/10	0	-1/35	0	-1/35	0	0
2	3	1	0	-3/70	0	-2/105	0	-5/231	0
3	3	1	-1/14	0	-2/105	0	-1/77	0	-50/3003

where $r_<$ and $r_>$ denote respectively the smaller and the greater of the two radius vectors, r_1 and r_2 , of the two electrons.

The electrostatic energy for the different terms belonging any configuration can now be written as

$$V_{(ne)SL} = V_{av} + V_t \quad (3-29)$$

where V_t for some of the simpler cases is as follows:

(i) All shells completely filled, or there is a single incompletely filled shell with either one electron or one hole. In these cases the configuration consists of a single term and,

$$V_t = 0$$

(ii) There is a single incompletely filled shell (designated by $n_1 l_1$) with m electrons

$$V_t = \sum_k f^k(l_1 SL) F^k(n_1 l_1, n_1 l_1)$$

Note that the screening parameters are functions of the partials of the Slater integrals F^k and G^k with respect to the appropriate screened nuclear charge γ_α , and F^k and G^k , which we evaluate using the hydrogenic wave function (Equation 3-12), are themselves functions of the screened

nuclear charges, and therefore of the screening parameter π_α 's. It is therefore readily seen that the right-hand side of Equation 2-20 is a non-linear function of all the screening parameters, $\pi_1, \pi_2, \dots, \pi_N$, when N is now the number of distinct subshells of electrons characterized by n and ℓ quantum numbers.

B.6 THE SLATER INTEGRALS

From Equations (B-26), (B-27) and (B-28) it is easy to see that F^k and G^k are symmetric in the two electrons. However, on account of the occurrence of $r_<$ and $r_>$ in this equation, it is necessary to break up the integral into two parts, which for the F integral we write as follows:

$$F^k(n_1\ell_1 n_2\ell_2; \gamma_1 \gamma_2) = F_1^k(n_1\ell_1 n_2\ell_2; \gamma_1 \gamma_2) + F_2^k(n_1\ell_1 n_2\ell_2; \gamma_1 \gamma_2) \quad (B-30)$$

with

$$F_1^k = \int_0^{\infty} P(n_2\ell_2 \gamma_2; r_2) \int_0^{r_2} P^k(n_1\ell_1 \gamma_1; r_1) dr_1 dr_2 \quad (B-31)$$

and

$$F_2^k = \int_0^{\infty} P^k(n_2\ell_2 \gamma_2; r_2) \int_{r_2}^{\infty} P(n_1\ell_1 \gamma_1; r_1) dr_1 dr_2 \quad (B-32)$$

where

$$P^k(n\ell\gamma; r) = r^k [P(n\ell\gamma; r)]^2 \quad (B-33)$$

Note that F_1^k and F_2^k are not symmetrical in the two electrons.

It is easy to prove that

$$F_2^k(n_1\ell_1 n_2\ell_2; \gamma_1 \gamma_2) = F_1^k(n_2\ell_2 n_1\ell_1; \gamma_2 \gamma_1) \quad (B-34)$$

For the G integral, these two parts turn out to be equal and we have

$$G^k(n_1\ell_1 n_2\ell_2; \gamma_1 \gamma_2) = 2 \int_0^\infty \int_0^{r_2} \frac{r_1^k}{r_2^{k+1}} \cdot P(n_1\ell_1; r_1) P(n_2\ell_2; r_2) P(n_1\ell_1; r_1) P(n_2\ell_2; r_2) dr_1 dr_2 \quad (B-35)$$

The calculations of the Slater F and G integrals, using hydrogenic wave functions, is extremely laborious, for electron shells whose wave functions possess more than one or two nodes. The author is not aware of any published work where these have been calculated as functions of the screened nuclear charges of the two electrons involved, nor are any general formulae for calculating them available in literature. We have, therefore, developed general formulae which are suitable for hand computations as well as computations using digital computers.

$$F^k(n_1\ell_1 n_2\ell_2; \gamma_1 \gamma_2) = Q_1^2 Q_2^2 (f_1^k - f_2^k + f_3^k) \quad (B-36)$$

where

$$f_1^k = \gamma_1^{-k} \gamma_2^{k+1} A_1^k A_2^{-k-1} \quad (B-37)$$

$$f_2^k = \frac{\gamma_1^{-k} \gamma_2^{2n_1+2n_2+k}}{(\gamma_1 + \gamma_2)^{2n_1+2n_2-1}} \cdot \sum_p \eta_p^k(n_1, l_1, n_2, l_2) \left(\frac{\gamma_1}{\gamma_2}\right)^p \quad (B-38)$$

$$f_3^k = f_2^{-k-1} \quad (B-39)$$

$$A_{np} = \sum_i^* \alpha_{np}^i (k+2l_1+i+2)! \quad (B-40)$$

$$\eta_p^k(n_1, l_1, n_2, l_2) = \sum_i^* \alpha_i^i (k+2l_1+i+2)! \cdot \sum_j^{\{2n_1+2n_2-1+k-p\}} \sum_t^{\{k+2l_1+i+2\}} \frac{\alpha_2^j (2l_2+j-k+t+1)! (2n_1+2n_2-1+k-j-t)!}{(p-t)! t! (2n_1+2n_2-1+k-j-p)!} \quad (B-41)$$

and α_{np}^p is defined by Equation (B-17). A symbol such as $\{a\}_b$ denotes the lesser of the two quantities inside the bracket.

$$G^k(n_1, l_1, n_2, l_2; \gamma_1, \gamma_2) = Q_1^2 Q_2^2 \sum_{j=0}^{2l_1+2l_2+6} \frac{\gamma_1^{2n_1+2n_2-2l_2-1} \gamma_2^{2l_2+3}}{(\gamma_1 + \gamma_2)^{2n_1+2n_2+1}} \sum_p^{\{2n_1+2n_2\}} \zeta_p^k(n_1, l_1, n_2, l_2) (\gamma_2 / \gamma_1)^p \quad (B-42)$$

where

$$\zeta_p^k(n_1, l_1, n_2, l_2) = \sum_{i,u}^* \sum_{j,v}^* \frac{d_1^u d_1^i d_2^v d_2^j}{2^{i+j+u+v}} \frac{(2n_1^*+2n_2^*-i-j-u-v)!}{(2n_1^*+2n_2^*-i-u-p)! (p-j-v)!} \quad (B-43)$$

$$\phi(\tau, D) = \tau! D! \left[1 - \frac{1}{2^{D+1}} \sum_{t=0}^{\tau} \binom{D+t}{D} \frac{1}{2^t} \right] \quad (B-44)$$

$$\tau = l_1 + l_2 + 2 + k + i + j \quad (B-45)$$

$$D = l_1 + l_2 + 1 - k + u + v \quad (B-46)$$

For the case of two equivalent electrons F^k and G^k are identical; we have the following simple expressions,

$$F^k(n l n l; \gamma_{ne} \gamma_{ne}) = \gamma_{ne}^4 2^D \sum_{q,p}^{2n^*} d_{ne}^p d_{ne}^q \phi(\tau, D) \quad (B-47)$$

where τ and D are now given by

$$\tau = 2l + 2 + k + p \quad (B-48)$$

and

$$D = 2l + 1 - k + q \quad (B-49)$$

and $\phi(\tau, D)$ is given by Equation (B-44).

A number of formulas using the above equations are given in Table B-3. Machine computations for η_p^k , η_p^{-k-1} and ζ_p^k have also been completed for all two electron combinations check marked in Table B-4.

TABLE B-3

SLATER INTEGRALS

(The formulae listed here are for $F^k(\alpha\beta; \chi_{\alpha\beta}^{-1})$ and $G^k(\alpha\beta; \chi_{\alpha\beta}^{-1})$, defined by Equation (B-50), where $\chi_{\alpha\beta} = \gamma_\alpha/\gamma_\beta$. The subscript $\alpha\beta$ are omitted for brevity.)

$$F^0(1s, 2s) = \frac{1}{4} \left[1 - (1+\chi)^{-5} (4\chi^3 + 3\chi + 1) \right]$$

$$F^0(1s, 2p) = \frac{1}{4} \left[1 - (1+\chi)^{-5} (3\chi + 1) \right]$$

$$F^0(1s, 3d) = \frac{1}{6} \left[1 - (1+\chi)^{-7} (4\chi + 1) \right]$$

$$F^0(3s, 3d) = \frac{1}{6} \left[1 - (1+\chi)^{-11} (412\chi^5 + 95\chi^4 + 138\chi^3 + 44\chi^2 + 10\chi + 1) \right]$$

$$F^0(2p, 3d) = \frac{1}{12} \left[2 - (1+\chi)^{-9} (60\chi^3 + 45\chi^2 + 15\chi + 2) \right]$$

$$F^2(2p, 3d) = \frac{\chi^{-2}}{12} \left[3 - (1+\chi)^{-9} (350\chi^5 + 378\chi^4 + 252\chi^3 + 108\chi^2 + 27\chi + 3) \right]$$

TABLE B-3 (continued)

$$F^o(3p, 3d) = \frac{1}{6} \left[1 - (1+\chi)^{-11} (300\chi^5 + 165\chi^4 + 110\chi^3 + 44\chi^2 + 10\chi + 1) \right]$$

$$F^2(3p, 3d) = \frac{\chi^{-2}}{3} \left[2 - (1+\chi)^{-11} (875\chi^7 + 847\chi^6 + 917\chi^5 + 660\chi^4 + 330\chi^3 + 110\chi^2 + 22\chi + 2) \right]$$

$$G^o(1s, 2s) = 2\chi^3(1+\chi)^{-7} (5\chi^2 - 15\chi + 13)$$

$$G^o(1s, 3s) = 2\chi^3(1+\chi)^{-9} (5\chi^4 - 30\chi^3 + 68\chi^2 - 62\chi + 21)$$

$$G^1(1s, 2p) = 14\chi^3(1+\chi)^{-7}$$

$$G^1(1s, 3p) = \frac{2}{3}\chi^3(1+\chi)^{-9} (56\chi^2 - 84\chi + 45)$$

TABLE B-3 (continued)

$$G^1(2s, 2p) = \chi^3(1+\chi)^{-9}(101\chi^2 - 70\chi + 14)$$

$$G^1(2s, 3p) = \frac{2}{3} \chi^3(1+\chi)^{-11}(404\chi^4 - 1430\chi^3 + 1598\chi^2 - 483\chi + 45)$$

$$G^2(1s, 3d) = 18 \chi^3(1+\chi)^{-9}$$

$$G^2(2s, 3d) = 2 \chi^3(1+\chi)^{-11}(124\chi^2 - 63\chi + 9)$$

$$G^2(3s, 3d) = \frac{2}{3} \chi^3(1+\chi)^{-13}(2477\chi^4 - 3598\chi^3 + 1892\chi^2 - 378\chi + 27)$$

$$G^1(2p, 3s) = 2 \chi^5(1+\chi)^{-11}(7\chi^4 - 70\chi^3 + 256\chi^2 - 360\chi + 187)$$

$$G^0(2p, 3p) = \frac{4}{3} \chi^5(1+\chi)^{-11}(186\chi^2 - 465\chi + 314)$$

$$G^2(2p, 3p) = \frac{20}{3} \chi^5(1+\chi)^{-11}(18\chi^2 - 45\chi + 35)$$

TABLE B-3 (continued)

$$G^1(2p, 3d) = 176 \chi^3 (1+\chi)^{-11}$$

$$G^3(2p, 3d) = \frac{308}{3} \chi^3 (1+\chi)^{-11}$$

$$G^1(3p, 3d) = \frac{4}{3} \chi^5 (1+\chi)^{-13} (1195 \chi^2 - 1232 \chi + 352)$$

$$G^3(3p, 3d) = \frac{4}{9} \chi^5 (1+\chi)^{-13} (2205 \chi^2 - 2156 \chi + 616)$$

TABLE B-4

THE TWO ELECTION COMBINATIONS FOR WHICH SLETER INTEGRALS HAVE BEEN CALCULATED
 (Marked by X. Because of symmetry, only the combinations above the diagonal are so marked.)

The set of simultaneous equations (E-20) contain partial derivatives of $F^k(\alpha, \beta)$ and $G^k(\alpha, \beta)$ with respect to γ_α as well as γ_β . Although $F^k(\alpha, \beta)$ and $G^k(\alpha, \beta)$ are symmetric in the two electrons α and β , their partials are not symmetric. From the preceding expressions for F^k and G^k the following general properties of these two integrals can be derived very simply,

$$R^k(\alpha\beta; \gamma_\alpha \gamma_\beta) = \gamma_\beta R^k(\alpha\beta; \chi_{\alpha\beta} - 1) \quad (E-50)$$

$$= \gamma_\alpha R^k(\alpha\beta; 1 - \chi_{\beta\alpha}) \quad (E-51)$$

where R stands for either integral F or G and

$$\chi_{\alpha\beta} = 1/\chi_{\beta\alpha} = \gamma_\alpha/\gamma_\beta = \frac{\gamma - \pi_\alpha}{\gamma - \pi_\beta} \quad (E-52)$$

The following expression for the partial derivatives are also derived easily,

$$\frac{\partial R^k(\alpha\beta; \gamma_\alpha \gamma_\beta)}{\partial \gamma_\alpha} = \frac{\partial R^k(\alpha\beta; \chi_{\alpha\beta} - 1)}{\partial \chi_{\alpha\beta}} \quad (E-53)$$

$$\frac{\partial R^k(\alpha\beta; \gamma_\alpha \gamma_\beta)}{\partial \gamma_\beta} = \frac{\partial R^k(\alpha\beta; 1 - \chi_{\beta\alpha})}{\partial \chi_{\beta\alpha}} \quad (E-54)$$

$$= R^k(\alpha\beta; \chi_{\alpha\beta} - 1) \quad (E-55)$$

$$- \frac{\partial R^k(\alpha\beta; \chi_{\alpha\beta} - 1)}{\partial \chi_{\alpha\beta}}$$

It is therefore clear that both partial derivatives of F and G integrals can be written as functions of a single parameter $\chi_{\alpha\beta}$.

The case for two equivalent electrons is a particularly simple one; the partial of $F^k(\alpha, \alpha)$ is merely a number, which is, in fact, the value of this integral for $\gamma_\alpha = \frac{2}{n_\alpha}$, the case of hydrogen atom (with atomic number unity).

3 THE SCREENING PARAMETERS

We now rewrite Equation (B-20) explicitly in terms of the partial derivatives of the Slater integrals

$$\Pi_{DSL} = 2(q_{0\alpha} - 1) \mathcal{F}(\alpha\alpha) + 4 \sum_{\beta \neq \alpha} \sum_k q_{0\beta} \cdot \left\{ f^k("l" SL) \mathcal{F}^k(\alpha\beta; \chi_{\alpha\beta}) + g^k("l" SL) \mathcal{G}^k(\alpha\beta; \chi_{\alpha\beta}) \right\} \quad (B-56)$$

where $\mathcal{F}(\alpha\alpha) = \sum_k f(l_\alpha l_\alpha) F^k(\alpha\alpha; 11) \quad (B-57)$

is merely a number, independent of any of the $\chi_{\alpha\beta}$'s,

$$\mathcal{F}^k(\alpha\beta; \chi_{\alpha\beta}) = \frac{\partial F^k(\alpha\beta; \gamma_\alpha \gamma_\beta)}{\partial \sum_\alpha} \quad (B-58)$$

and

$$\mathcal{G}^k(\alpha\beta; \chi_{\alpha\beta}) = \frac{\partial G^k(\alpha\beta; \gamma_\alpha \gamma_\beta)}{\partial \gamma_\alpha} \quad (B-59)$$

$f^k("l" SL)$ and $g^k("l" SL)$ denote the coefficients in which the SL dependent contributions to the electrostatic energy are explicitly included. The symbol " l " denotes the orbital quantum numbers of all the incompletely filled shells including the parentages, etc.

We note that,

$$\chi_{\alpha\beta} = \frac{\frac{2}{n_\alpha} Z - \pi_\alpha}{\frac{2}{n_\beta} Z - \pi_\beta} \quad (B-60)$$

and for the case $Z \rightarrow \infty$

$$\chi_{\alpha\beta} \rightarrow \chi_{\alpha\beta}^\infty = \frac{n_\beta}{n_\alpha} \quad (B-61)$$

The method for computing the screening parameters is as follows.

We first calculate a set of π 's with $\chi_{\alpha\beta} = \frac{n_\beta}{n_\alpha}$. We call these asymptotic π 's or π^∞ . With these π^∞ 's, and some suitably chosen large value of Z , we compute a new set of $\chi_{\alpha\beta}$, and use these to recalculate π 's by iteration. We then decrease Z by successive steps and keep repeating the same iterative procedure. Thus we work along an iso-electronic sequence and obtain the screening parameters for any desired number of atoms and ions belonging to this iso-electronic sequence. Since the procedure is very time consuming, a program for computations on a digital computer has been developed.

The asymptotic screening constants for two electron combinations, and using the average energy of a configuration only, can however be computed quite easily. They are defined as follows:

$$\begin{aligned} \pi^\infty(\alpha, \beta) = \sum_k & \left[f^k(l_\alpha l_\beta) \bar{f}^k(\alpha\beta; \chi_{\alpha\beta}^\infty) \right. \\ & \left. + g^k(l_\alpha l_\beta) \bar{g}^k(\alpha\beta; \chi_{\alpha\beta}^\infty) \right] \quad (B-62) \end{aligned}$$

for $\alpha \neq \beta$

and

$$\pi^\infty(\alpha, \alpha) = \bar{f}(\alpha\alpha) \quad (B-63)$$

The asymptotic screening constants for the average energy of a configuration can then be constructed from these two electron screening constants as follows:

$$\Pi_{\alpha}^{\infty} = \frac{4}{\alpha} \sum_{\beta} q_{\alpha \beta} \pi^{\infty}(\alpha, \beta) \quad (B-64)$$

B.8 THE CALCULATION OF THE TRANSITION INTEGRALS

The only case of interest for an electric dipole transition is when the azimuthal quantum number of the active electron changes by one unit. Therefore, the calculation of the following integral is of sufficient generality:

$$\begin{aligned} I_1(n_1, l_1, n_2, l_1-1; \gamma_1, \gamma_2) &= \int_0^{\infty} P(n_1, l_1; r) P(n_2, l_1-1; r) r dr \\ &= Q_1 Q_2 \gamma_1^{\frac{l_1+1}{2}} \gamma_2^{\frac{l_1-1}{2}} J_{2l_1+2}^{1,2}(-n_1^*, -n_2^*) \end{aligned} \quad (B-65)$$

where

$$\begin{aligned} J_{\gamma}^{s, p}(-n_1^*, -n_2^*) &= \int_0^{\infty} \exp\left[-\frac{1}{2}(\gamma_1 + \gamma_2)r\right] r^{s-1-p} \\ &\cdot F_1(-n_1^*, s; \gamma_1 r) F_1(-n_2^*, s-p; \gamma_2 r) \end{aligned} \quad (B-66)$$

A similar integral with $\gamma_1 = \frac{2}{n_1}$, $\gamma_2 = \frac{2}{n_2}$ has been evaluated by Gordon^(B-26).

The necessary formulas for the evaluation of integrals involving confluent hypergeometric functions have been given, among other, by Landau and Lifshitz^(B-27) in their mathematical appendix.

The p index can be reduced by using the formula

$$J_{\gamma}^{s,p}(-n_1^*, -n_2^*) = \frac{\gamma-1}{\gamma} \left\{ J_{\gamma-1}^{s,p-1}(-n_1^*, -n_2^*) - J_{\gamma-1}^{s,p-1}(-n_1^*-1, n_2^*) \right\} \quad (B-67)$$

whereas the s index can be reduced by using another formula

$$\begin{aligned} J_{\gamma}^{s+1,0}(-n_1^*, -n_2^*) &= \frac{4}{\gamma_1^2 - \gamma_2^2} \left\{ \left[\frac{1}{2} \gamma (\gamma_1 - \gamma_2) + \gamma_1 n_1^* - \gamma_2 n_2^* - \gamma_2 s \right] J_{\gamma}^{s,0}(-n_1^*, -n_2^*) \right. \\ &\quad \left. + s(\gamma-1+s+2n_2^*) J_{\gamma}^{s-1,0}(-n_1^*, -n_2^*) - 2n_2^* s J_{\gamma}^{s-1,0}(-n_1^*, -n_2^*+1) \right\} \quad (B-68) \end{aligned}$$

Successive applications of Equations (B-67) and (B-68) to (B-66) yield

$$\begin{aligned} J_{2\ell+2}^{1,2}(-n_1^*, -n_2^*) &= \frac{2\ell(2\ell+1)}{\gamma_1^2} \frac{4}{(\gamma_1^2 - \gamma_2^2)} \left\{ \left[\gamma_1(\ell+n_1^*) - \gamma_2(\ell+n_2^*) \right] \right. \\ &\quad \left. + J_{2\ell}^{0,0}(-n_1^*, -n_2^*) - 2[\gamma_1(\ell+n_1^*+1) - \gamma_2(\ell+n_2^*)] J_{2\ell}^{0,0}(-n_1^*-1, -n_2^*) \right\} \quad (B-69) \end{aligned}$$

$$+ \left[\gamma_1(\ell+n_1^*+2) - \gamma_2(\ell+n_2^*) \right] J_{2\ell}^{0,0}(-n_1^*-2, n_2^*) \}$$

$J_{2\ell}^{0,0}$ can be evaluated in closed form by another formula

$$J_{\gamma}^{0,0}(\alpha_1, \alpha_2) = (-1)^{-\alpha_2} \frac{\gamma}{2} \Gamma(\gamma) (\gamma_2 + \gamma_1)^{\alpha_1 + \alpha_2 - \gamma} (\gamma_2 - \gamma_1)^{-\alpha_1 - \alpha_2} \quad (B-70)$$

$$\cdot {}_2F_1(\alpha_1, \alpha_2; \gamma; -4\gamma_1\gamma_2 / (\gamma_2 - \gamma_1)^2)$$

where ${}_2F_1$ is a hypergeometric function given, in general, by

$$\begin{aligned} {}_2F_1(a, b; c; \mu) &= 1 + \frac{a b}{c 1!} \mu + \frac{a(a+1) b(b+1)}{c(c+1) 2!} \mu^2 \\ &\quad + \frac{a(a+1)(a+2) b(b+1)(b+2)}{c(c+1)(c+2) 3!} \mu^3 + \dots \end{aligned} \quad (B-71)$$

The series terminates after a finite number of terms when a and/or b are negative integers. On substitution of (B-70) in (B-69) and simplification we get

$$\begin{aligned} J_{2l+2}^{1,2}(-n_1^*, -n_2^*) &= (-1)^{n_2^*+1} (2l+1)! \frac{2^{l+2}}{2} \frac{(y_2-y_1)^{n_1+n_2-2l-2}}{y_1^2 (y_2+y_1)^{n_1+n_2}} \\ &\cdot \left\{ (y_1 n_1 - y_2 n_2 - y_1) {}_2F_1(-n_1^*) - 2(y_1 n_1 - y_2 n_2) \frac{y_2 - y_1}{y_2 + y_1} \right. \\ &\quad \left. \cdot {}_2F_1(-n_1^*-1) + (y_1 n_1 - y_2 n_2 + y_1) \left(\frac{y_2 - y_1}{y_2 + y_1} \right)^2 {}_2F_1(-n_1^*-2) \right\} \end{aligned} \quad (B-72)$$

where

$${}_2F_1(\alpha) \equiv F(\alpha, -n_2^*; 2l; -\frac{4y_1 y_2}{(y_2 - y_1)^2}) \quad (B-73)$$

The following relation may be used to reduce the number of hypergeometric functions from three to two in (B-72), if desired.

$$(c - 2a - (b - a)\mu) {}_2F_1(a) + a(1 - \mu) {}_2F_1(a+1) - (c - a) {}_2F_1(a-1) \quad (B-74)$$

where

$${}_2F_1(a) \equiv {}_2F_1(a, b; c; \mu)$$

Combining (B-65) with (B-72) we get

$$\begin{aligned} I_1(n_1, l, n_2, l-1; y_1, y_2) &= (-1)^{n_2^*+1} Q_1 Q_2 (2l+1)! \frac{2^{l+2}}{2} y_1^{l-\frac{1}{2}} y_2^{l+\frac{1}{2}} \\ &\cdot \frac{(y_2 - y_1)^{n_1+n_2-2l-2}}{(y_2 + y_1)^{n_1+n_2}} \left\{ (y_1 n_1 - y_2 n_2 - y_1) {}_2F_1(-n_1^*) \right. \\ &\quad \left. - 2(y_1 n_1 - y_2 n_2) \frac{y_2 - y_1}{y_2 + y_1} {}_2F_1(-n_1^*-1) \right. \\ &\quad \left. + (y_1 n_1 - y_2 n_2 + y_1) \left(\frac{y_2 - y_1}{y_2 + y_1} \right)^2 {}_2F_1(-n_1^*-2) \right\} \end{aligned} \quad (B-75)$$

which for the special case $\gamma_1 = \frac{2}{n_1}, \gamma_2 = \frac{2}{n_2}$, reduces to the following equation first derived by Gordon (B-26).

$$I_1(n_1, l, n_2, l-1) = (-1)^{n_2^*} \left[\frac{(n_1+l)! (n_2+l-1)!}{(n_1-l-1)! (n_2-l)!} \right] \frac{(4n_1 n_2)^{l+1}}{4(2l-1)!} \cdot \frac{(n_1-n_2)^{n_1-n_2-2l-2}}{(n_1+n_2)^{n_1+n_2}} \left\{ {}_2F_1 \left(-n_1^*, -n_2^*; 2l; -\frac{4n_1 n_2}{(n_1-n_2)^2} \right) \right. \\ \left. - \left(\frac{n_1-n_2}{n_1+n_2} \right)^2 {}_2F_1 \left(-n_1^* - 2, -n_2^*; 2l; -\frac{4n_1 n_2}{(n_1-n_2)^2} \right) \right\} \quad (B-76)$$

The following special cases can be obtained easily

$$I_1(np, 1s; \gamma_1, \gamma_2) = 32(n^2-1)^{1/2} \gamma_1^{5/2} \gamma_2^{3/2} \left[\frac{(3\gamma_2 - \gamma_1)^{n-3}}{(3\gamma_2 + \gamma_1)^{n+3}} \right] \quad (B-77)$$

$$I_1(np, 2s; \gamma_1, \gamma_2) = 32(n^2-1)^{1/2} \gamma_1^{5/2} \gamma_2^{3/2} \left[n \gamma_1^3 - 2 \gamma_1^2 \gamma_2 (n+2) \right. \\ \left. + 9n \gamma_1 \gamma_2^2 - 8 \gamma_2^3 \right] \frac{(3\gamma_2 - \gamma_1)^{n-4}}{(3\gamma_2 + \gamma_1)^{n+4}} \quad (B-78)$$

$$I_1(nd, 2p; \gamma_1, \gamma_2) = \frac{64(n^4 - 5n^2 + 4)^{1/2}}{3^{4/2}} \gamma_1^{7/2} \gamma_2^{5/2} \\ \cdot (3\gamma_2 - n\gamma_1) \frac{(3\gamma_2 - \gamma_1)^{n-4}}{(3\gamma_2 + \gamma_1)^{n+4}} \quad (B-79)$$

$$I_1(2p, ns; \gamma_1, \gamma_2) = (-1)^{n+1} \frac{64}{3^{4/2}} \gamma_1^{5/2} \gamma_2^{3/2} \left[n(2+n)^2 \gamma_2^3 \right. \\ \left. - 3(1+2n^2) \gamma_2 \gamma_1 + 9n \gamma_2 \gamma_1^2 - 3 \gamma_1^3 \right] \\ \cdot \frac{(3\gamma_2 - \gamma_1)^{n-4}}{(3\gamma_2 + \gamma_1)^{n+4}} \quad (B-80)$$

B.9 ALTERNATE EXPRESSION FOR TRANSITION INTEGRALS

For the sake of generality we shall evaluate the following

integral,

$$I_p^q(n_1 l_1 n_2 l_2; \gamma_1 \gamma_2) = \int_0^\infty P(n_1 l_1; r) P(n_2 l_2; r) \cdot r^p \exp[-qr] dr \quad (B-81)$$

For Coulomb potential wave functions, we shall later put q equal to zero. p equals unity for the electric dipole case, and it equals 2, 3, 4, etc. for higher multipole cases. Substituting from Equation (B-12) we get,

$$I_p^q(n_1 l_1 n_2 l_2; \gamma_1 \gamma_2) = Q_1 Q_2 \gamma_1^{l_1 + \frac{3}{2}} \gamma_2^{l_2 + \frac{3}{2}} \int_0^\infty r^{l_1 + l_2 + p + 2} \cdot \exp[-\frac{1}{2}(\gamma_1 + \gamma_2 + 2q)r] \cdot F_1(-n_1^*, 2l_1 + 2; \gamma_1 r) F_1(-n_2^*, 2l_2 + 2; \gamma_2 r) dr. \quad (B-82)$$

This integration can be performed using certain standard results in the theory of confluent hypergeometric functions, (see for example Slater^(B-28), page 54). Performing the integration we obtain,

$$I_p^q = Q_1 Q_2 2^{l_1 + l_2 + 3 + p} (l_1 + l_2 + 2 + p)! \frac{\gamma_1^{l_1 + \frac{3}{2}} \gamma_2^{l_2 + \frac{3}{2}}}{(3\gamma_1 + 3\gamma_2 + 2q)^{l_1 + l_2 + 3 + p}} \cdot \sum_i \frac{n_1^* [(-i)^i (n_1^*)! (2l_1 + i)!]}{(n_1^* - i)! (2l_1 + 1 + i)! i!} \frac{(3\gamma_1 + 3\gamma_2 + 2q)^{l_1 + l_2 + 2 + p + i}}{(l_1 + l_2 + 2 + p + i)!} \cdot \left(\frac{2\gamma_1}{\gamma_1 + \gamma_2 + 2q} \right)^i F_1(-n_2^*, l_1 + l_2 + 3 + p + i; 2l_2 + 2; \frac{2\gamma_2}{\gamma_1 + \gamma_2 + 2q}) \quad (B-83)*$$

*A similar result has also been obtained by Prof. D. H. Menzel (unpublished).

where the expression in the square bracket following the summation sign can be readily seen to be equal to d_1^i . ${}_2F_1$ is the hypergeometric function defined by Equation (B-71). The computation of the expression on the right hand side of the above equation is quite straight forward in principle, but becomes very laborious as n_1^* and n_2^* become large.

We shall now proceed on to the special case we are interested in, namely the case where $p = 1$ and $q = 0$. For this case,

$$\begin{aligned}
 & {}_2F_1(-n_1^*, l_1 + l_2 + 4 + i; 2l_2 + 2; \frac{2\gamma_2}{\gamma_1 + \gamma_2}) \\
 &= \sum_j^{\infty} (-1)^j \frac{(n_2^*)! (2l_2 + i)!}{(n_2^* - j)! (2l_2 + 1 + j)! j!} \\
 & \cdot \frac{(l_1 + l_2 + 3 + i + j)!}{(l_1 + l_2 + 3 + i)!} \left(\frac{2\gamma_2}{\gamma_1 + \gamma_2}\right)^j \\
 &= \sum_j^{\infty} d_1^j d_2^j \frac{(l_1 + l_2 + 3 + i + j)!}{(l_1 + l_2 + 3 + i)!} \left(\frac{2\gamma_2}{\gamma_1 + \gamma_2}\right)^j
 \end{aligned} \tag{B-84}$$

and

$$I_1(n_1, n_2, l_1; \gamma_1, \gamma_2) = Q_1 Q_2 \frac{\gamma_1^{l_1 + l_2 + 4}}{\gamma_1^{l_1 + 3} \gamma_2^{l_2 + 3}} \frac{\gamma_2^{l_1 + l_2 + 4}}{(\gamma_1 + \gamma_2)^{l_1 + l_2 + 4}} \mathcal{J} \tag{B-85}$$

where

$$\mathcal{J} = \sum_i^{\infty} \sum_j^{\infty} d_1^i d_2^j 2^{i+j} (l_1 + l_2 + 3 + i + j)! \cdot \frac{\gamma_1^i \gamma_2^j}{(\gamma_1 + \gamma_2)^{i+j}} \tag{B-86}$$

Needless to say that the same expressions can also be obtained by integration of Equation (B-81) with the radial wave functions given by Equation (B-12) combined with Equation (B-14). Some further simplifications of the above expression can be brought about as follows. The common denominator of all the terms under the two summations is $(\gamma_1 + \gamma_2)^{n_1^* + n_2^*}$. Taking the common denominator and performing binomial expansion of the resulting term, namely $(\gamma_1 + \gamma_2)^{n_1^* + n_2^* - i - j}$, we obtain

$$J = \frac{\gamma_1^{n_1^* + n_1^*}}{(\gamma_1 + \gamma_2)^{n_1^* + n_2^*}} \sum_i \sum_j \sum_p \frac{(n_1^* + n_2^* - i - j)!}{d_1^i d_2^j} 2^{i+j} \cdot (l_1 + l_2 + 3 + i + j)! \cdot \frac{(n_1^* + n_2^* - i - j)!}{(n_1^* + n_2^* - i - j - p)! p!} \left(\frac{\gamma_2}{\gamma_1}\right)^{p+j} \quad (B-87)$$

Replacing p by another index u , such that $u = p + j$, we get,

$$J = \frac{\gamma_1^{n_1^* + n_1^*}}{(\gamma_1 + \gamma_2)^{n_1^* + n_2^*}} \sum_i \sum_j \sum_{u=j}^{n_1^* + n_2^*} \frac{(n_1^* + n_2^* - i)!}{d_1^i d_2^j} 2^{i+j} \cdot (l_1 + l_2 + 3 + i + j)! \cdot \frac{(n_1^* + n_2^* - i - j)!}{(n_1^* + n_2^* - i - u)! (u - j)!} \left(\frac{\gamma_2}{\gamma_1}\right)^u \quad (B-88)$$

$$= \sum_{u=0}^{n_1^* + n_2^*} \Psi^u(n_1, l_1, n_2, l_2) \frac{\gamma_1^{n_1^* + n_2^* - u}}{(\gamma_1 + \gamma_2)^{n_1^* + n_2^*}} \frac{\gamma_2^u}{(\gamma_1 + \gamma_2)^{n_1^* + n_2^*}}$$

where

$$\Psi^u(n_1 l_1, n_2 l_2) = \sum_i \frac{\{n_1^*\}}{\{n_1^* + n_2^* - u\}} \frac{\{n_2^*\}}{\sum_j} \frac{d_1^i d_2^j}{2^{i+j}}$$

$$\cdot (l_1 + l_2 + i + j)! \frac{(n_1^* + n_2^* - i - j)!}{(n_1^* + n_2^* - i - u)! (u - j)!} \quad (B-89)$$

u takes on all integral values from 0 to $(n_1^* + n_2^*)$. Ψ^u is a function of the quantum numbers of the two electrons under consideration, but it is independent of the screened nuclear charges, γ_1 and γ_2 . When n_1^* and n_2^* are so large that desk calculations are too tedious, the calculation of Ψ^u on electronic computers is a trivial matter, giving us analytical expressions of I_1 in terms of Ψ^u as follows,

$$I_1(n_1 l_1, n_2 l_2; \gamma_1, \gamma_2) = Q_1 Q_2 2^{l_1 + l_2 + 4} \cdot \frac{\gamma_1^{l_1 + \frac{3}{2}} \gamma_2^{l_2 + \frac{3}{2}}}{(\gamma_1 + \gamma_2)^{n_1 + n_2 + 2}} \cdot \sum_u \frac{(n_1^* + n_2^*)}{\Psi^u(n_1 l_1, n_2 l_2)} \gamma_1^{n_1^* + n_2^* - u} \gamma_2^u \quad (B-90)$$

It should be noted that whereas I_1 is a symmetric function of the two electrons, Ψ^u is not.

Table 2-5 gives expressions for I_1 for a selected number of transitions.

TABLE B-5 DIPOLE INTEGRALS

$$I_1(2p,1o) = \frac{64(3)^{\frac{1}{2}} \delta_1^{\frac{3}{2}} \delta_2^{\frac{1}{2}}}{(\delta_1 + \delta_2)^5}$$

$$I_1(3p,1o) = \frac{64(2)^{\frac{1}{2}} \delta_1^{\frac{5}{2}} \delta_2^{\frac{1}{2}}}{(\delta_1 + \delta_2)^6} (2\delta_2 - 3\delta_1)$$

$$I_1(4p,1o) = \frac{64(15)^{\frac{1}{2}} \delta_1^{\frac{7}{2}} \delta_2^{\frac{1}{2}}}{(\delta_1 + \delta_2)^7} (\delta_2 - 2\delta_1)(\delta_2 - \delta_1)$$

$$I_1(5p,1o) = \frac{64(6)^{\frac{1}{2}} \delta_1^{\frac{9}{2}} \delta_2^{\frac{1}{2}}}{(\delta_1 + \delta_2)^8} (2\delta_2 - 5\delta_1)(\delta_2 - \delta_1)^3$$

$$I_1(6p,1o) = \frac{64(35)^{\frac{1}{2}} \delta_1^{\frac{11}{2}} \delta_2^{\frac{1}{2}}}{(\delta_1 + \delta_2)^9} (\delta_2 - 3\delta_1)(\delta_2 - \delta_1)^5$$

TABLE B-5 (cont.)

$$I_1(7p,1o) = \frac{128(3)^{1/2} \bar{z}_1^{5/2} \bar{z}_2^{3/2}}{(\bar{z}_1 + \bar{z}_2)^6} (2\bar{z}_2 - 7\bar{z}_1)(\bar{z}_2 - \bar{z}_1)^4$$

$$I_1(2p,2o) = 64(3)^{1/2} \frac{\bar{z}_1^{5/2} \bar{z}_2^{3/2}}{(\bar{z}_1 + \bar{z}_2)^6} (\bar{z}_1 - 4\bar{z}_2)$$

$$I_1(3p,2o) = \frac{64(2)^{1/2}}{(\bar{z}_1 + \bar{z}_2)^7} \left[-3\bar{z}_1^2 + 19\bar{z}_1\bar{z}_2 - 8\bar{z}_2^2 \right]$$

$$I_1(4p,2o) = \frac{32(15)^{1/2} \bar{z}_1^{5/2} \bar{z}_2^{3/2}}{(\bar{z}_1 + \bar{z}_2)^8} \left[4\bar{z}_1^3 - 36\bar{z}_1^2\bar{z}_2 + 36\bar{z}_1\bar{z}_2^2 - 8\bar{z}_2^3 \right]$$

$$I_1(5p,2o) = \frac{64(6)^{1/2} \bar{z}_1^{5/2} \bar{z}_2^{3/2}}{(\bar{z}_1 + \bar{z}_2)^9} (\bar{z}_2 - \bar{z}_1) \left[5\bar{z}_1^3 - 54\bar{z}_1^2\bar{z}_2 + 45\bar{z}_1\bar{z}_2^2 - 8\bar{z}_2^3 \right]$$

$$I_1(6p,2o) = \frac{32(35)^{1/2} \bar{z}_1^{5/2} \bar{z}_2^{3/2}}{(\bar{z}_1 + \bar{z}_2)^{10}} (\bar{z}_2 - \bar{z}_1)^2 \left[6\bar{z}_1^3 - 76\bar{z}_1^2\bar{z}_2 + 54\bar{z}_1\bar{z}_2^2 - 8\bar{z}_2^3 \right]$$

$$I_1(7p,2o) = \frac{128(3)^{1/2} \bar{z}_1^{5/2} \bar{z}_2^{3/2}}{(\bar{z}_1 + \bar{z}_2)^{11}} (\bar{z}_2 - \bar{z}_1)^3 \left[7\bar{z}_1^3 - 102\bar{z}_1^2\bar{z}_2 + 63\bar{z}_1\bar{z}_2^2 - 8\bar{z}_2^3 \right]$$

TABLE B-5 (cont.)

$$I_{1}(2p,3o) = -\frac{32 \cdot 3^{\frac{1}{2}} \cdot 3^{\frac{1}{2}}}{(3)^{\frac{1}{2}} (3_1 + 3_2)^{\frac{1}{2}}} (3_2 - 3_1)^{-1} \left[(23_1 - 33_2)(33_1^2 + 193_1^3 - 183_13_2) \right. \\ \left. - 3_2(93_1^2 + 93_1^3 - 223_13_2) \right]$$

$$I_{1}(2p,4o) = \frac{32 \cdot 3^{\frac{1}{2}} \cdot 3^{\frac{1}{2}}}{(3)^{\frac{1}{2}} (3_1 + 3_2)^{\frac{1}{2}}} \left[(23_1 - 43_2)(33_1^2 + 333_1^3 - 243_13_2) - 3_2(123_1^2 + 123_1^3 - 363_13_2) \right]$$

$$I_{1}(2p,5o) = -\frac{32 \cdot 3^{\frac{1}{2}} \cdot 3^{\frac{1}{2}} (3_2 - 3_1)}{(3)^{\frac{1}{2}} (3_1 + 3_2)^{\frac{1}{2}}} \left[(23_1 - 53_2)(33_1^2 + 263_1^3 - 303_13_2) - 3_2(153_1^2 + 153_1^3 - 543_13_2) \right]$$

$$I_{1}(3p,5o) = \frac{128 (3)^{\frac{1}{2}} \cdot 3^{\frac{1}{2}} \cdot 3^{\frac{1}{2}}}{(3_1 + 3_2)^{\frac{1}{2}}} \left[(3_1 + 3_2)^5 - \frac{1}{2}(3_1 + 3_2)(3_1 + 3_2)^4 + 6(3_13_1 + 23_2)(3_13_2)^3 \right. \\ \left. - 140(3_13_2^2 + 23_2^3)(3_1 + 3_2)^2 + 224(53_13_1^2 + 3_1^3)(3_1 + 3_2) \right. \\ \left. - 8963_13_2^4 \right]$$

TABLE B-5 (cont.)

$$I_1(4p, 5s) = \frac{64(5)^4 \delta_1^4 \delta_2^4}{(\delta_1 + \delta_2)^9} \left[(\delta_1 + \delta_2)^6 - 5(\delta_1 + 4\delta_2)(\delta_1 + \delta_2)^5 + 6(\delta_1^5 + 20\delta_1^4 + 20\delta_1^3)(\delta_1 + \delta_2)^4 \right.$$

$$- 56(3\delta_1^2 \delta_2 + 15\delta_1 \delta_2^2 + 5\delta_1^3)(\delta_1 + \delta_2)^3$$

$$+ 224(6\delta_1^3 \delta_2^2 + 10\delta_1 \delta_2^3 + \delta_2^4)(\delta_1 + \delta_2)^2$$

$$\left. - 2016(2\delta_1^2 \delta_2^3 + \delta_1 \delta_2^4)(\delta_1 + \delta_2) + 4032\delta_1^2 \delta_2^4 \right]$$

$$I_1(5p, 5s) = \frac{128(6)^4 \delta_1^4 \delta_2^4}{(\delta_1 + \delta_2)^9} \left[(\delta_1 + \delta_2)^7 - \frac{5}{2}(3\delta_1 + 8\delta_2)(\delta_1 + \delta_2)^6 + 30(3\delta_1^2 + 6\delta_1 \delta_2 + 4\delta_2^2)(\delta_1 + \delta_2)^5 \right.$$

$$- 70(3\delta_1^3 + 12\delta_1^2 \delta_2 + 18\delta_1 \delta_2^2 + 4\delta_2^3)(\delta_1 + \delta_2)^4$$

$$+ 224(3\delta_1^4 + 15\delta_1^3 \delta_2 + 30\delta_1^2 \delta_2^2 + 10\delta_2^3)(\delta_1 + \delta_2)^3$$

$$- 1008(3\delta_1^2 \delta_2 + 20\delta_1^3 \delta_2^2 + 20\delta_1^2 \delta_2^3)(\delta_1 + \delta_2)^2$$

$$\left. + 6720(3\delta_1^4 \delta_2^2 + 10\delta_1^3 \delta_2^3)(\delta_1 + \delta_2) - 73920\delta_1^4 \delta_2^4 \right]$$

TABLE B-5 (cont.)

$$I(6p, 5o) = \frac{64(35)^{\frac{1}{2}} 3^{\frac{1}{2}} 5^{\frac{1}{2}}}{(3_1 + 3_2)^{13}} \left[(3_1 + 3_2)^6 - 10(3_1 + 23_2)(3_1 + 3_2)^5 + 12(103_2 + 203_1 + 33_2^2)(3_1 + 3_2)^4 \right. \\ - 56(53_2^3 + 303_2^23_1 + 183_23_1^2 + 3_1^3)(3_1 + 3_2)^3 \\ + 32(73_2^4 + 1403_2^33_1 + 2523_2^23_1^2 + 563_23_1^3 + 3_1^4)(3_1 + 3_2)^2 \\ - 576(73_2^43_1 + 423_2^33_1^2 + 283_2^23_1^3 + 23_23_1^4)(3_1 + 3_2)^2 \\ + 384(63_2^43_1^2 + 1403_2^33_1^3 + 303_2^23_1^4)(3_1 + 3_2)^2 \\ \left. - 8448(73_2^43_1^3 + 53_2^33_1^4)(3_1 + 3_2) + 506083_1^53_2^2 \right]$$

$$I(2p, 6o) = \frac{32(3_1^{\frac{1}{2}} 3_2^{\frac{1}{2}})^{\frac{1}{2}}(3_1 - 3_2)^{\frac{1}{2}}}{(3_1 + 3_2)^{10}} \left[(23_1 - 63_2)(33_1^2 + 373_2^2 - 363_13_2) - 3_2(193_1^2 + 163_2^2 - 73_13_2) \right]$$

TABLE B - 5 (cont.)

$$\begin{aligned}
 I(4_P, 6_S) = & \frac{64(15)^4 j_1^2 j_2^2}{(j_1 + j_2)^5} \left[(j_1 + j_2)^7 - 5(j_1 + 5j_2)(j_1 + j_2)^6 \right. \\
 & + 2(3j_1^2 + 75j_1 j_2 + 100j_2^2)(j_1 + j_2)^5 \\
 & - 70(3j_1^2 j_2 + 20j_1 j_2^2 + 10j_2^3)(j_1 + j_2)^4 \\
 & + 1120(2j_1^4 j_2^2 + 5j_1^2 j_2^4 + j_2^6)(j_1 + j_2)^3 \\
 & - 672(15j_1^2 j_2^3 + 15j_1 j_2^5 + j_2^7)(j_1 + j_2)^2 \\
 & \left. + 6720(3j_1^2 j_2^4 + j_1 j_2^5)(j_1 + j_2) - 14784 j_1^5 j_2^5 \right]
 \end{aligned}$$

TABLE B -5 (cont.)

$$\begin{aligned}
 I(5p, 6s) = & \frac{120(6) \cdot 3^4 \cdot 5^4}{(3_1 + 3_2)^{13}} \left[(3_1 + 3_2)^8 - \frac{5}{2}(3_1 + 103_2)(3_1 + 3_2)^7 \right. \\
 & + (183_1 + 2253_13_2 + 2003_2^2)(3_1 + 3_2)^6 \\
 & - 14(3_1^3 + 453_1^23_2 + 1503_13_2^2 + 503_2^3)(3_1 + 3_2)^5 \\
 & + 560(23_1^33_2 + 123_1^23_2^2 + 153_13_2^3 + 23_2^4)(3_1 + 3_2)^4 \\
 & - 336(203_1^33_2^2 + 903_1^23_2^3 + 453_13_2^4 + 23_2^5)(3_1 + 3_2)^3 \\
 & + 3360(53_1^33_2^3 + 183_1^23_2^4 + 33_13_2^5)(3_1 + 3_2)^2 \\
 & - 2464(303_1^33_2^4 + 33_13_2^5)(3_1 + 3_2) \\
 & \left. + 591363_1^33_2^5 \right]
 \end{aligned}$$

TABLE B-5 (cont.)

$$\begin{aligned}
 I(6p, 6s) = & \frac{64(35)^4 \bar{z}_1^2 \bar{z}_2^2}{(\bar{z}_1 + \bar{z}_2)^4} \left[\left(\bar{z}_2 + \bar{z}_1 \right)^6 - 5(5\bar{z}_2 + \bar{z}_1)(\bar{z}_2 + \bar{z}_1)^4 \right. \\
 & + 4(50\bar{z}_2^2 + 75\bar{z}_2\bar{z}_1 + 9\bar{z}_1^2)(\bar{z}_2 + \bar{z}_1)^3 \\
 & - 28(25\bar{z}_2^3 + 150\bar{z}_2^2\bar{z}_1 + 45\bar{z}_2\bar{z}_1^2 + 2\bar{z}_1^3)(\bar{z}_2 + \bar{z}_1)^6 \\
 & + 32(35\bar{z}_2^4 + 350\bar{z}_2^3\bar{z}_1 + 420\bar{z}_2^2\bar{z}_1^2 + 70\bar{z}_2\bar{z}_1^3 + \bar{z}_1^4)(\bar{z}_2 + \bar{z}_1)^5 \\
 & - 96(7\bar{z}_2^5 + 52.5\bar{z}_2^4\bar{z}_1 + 630\bar{z}_2^3\bar{z}_1^2 + 280\bar{z}_2^2\bar{z}_1^3 + 15\bar{z}_2\bar{z}_1^4 + \bar{z}_1^5)(\bar{z}_2 + \bar{z}_1)^4 \\
 & + 1920(7\bar{z}_2^6 + 63\bar{z}_2^5\bar{z}_1 + 70\bar{z}_2^4\bar{z}_1^2 + 10\bar{z}_2^3\bar{z}_1^3)(\bar{z}_2 + \bar{z}_1)^3 \\
 & - 4224(21\bar{z}_2^7\bar{z}_1 + 70\bar{z}_2^6\bar{z}_1^2 + 25\bar{z}_2^5\bar{z}_1^3)(\bar{z}_2 + \bar{z}_1)^2 \\
 & + 16896(14\bar{z}_2^8\bar{z}_1^3 + 15\bar{z}_2^7\bar{z}_1^4)(\bar{z}_2 + \bar{z}_1) \\
 & \left. - 219648 \bar{z}_1^5 \bar{z}_2^4 \right]
 \end{aligned}$$

TABLE B-5 (cont.)

$$I(3d, 2p) = \frac{384(10)^{1/2} \gamma_1^{3/2} \gamma_2^{5/2}}{(3)^{1/2} (\gamma_1 + \gamma_2)^3}$$

$$I(4d, 2p) = \frac{384(5)^{1/2} \gamma_1^{3/2} \gamma_2^{5/2}}{(3)^{1/2} (\gamma_1 + \gamma_2)^3} (3\gamma_2 - 4\gamma_1)$$

$$I(5d, 2p) = \frac{384(14)^{1/2} \gamma_1^{3/2} \gamma_2^{5/2}}{(3)^{1/2} (\gamma_1 + \gamma_2)^3} (\gamma_2 - \gamma_1)(3\gamma_2 - 5\gamma_1)$$

$$I(6d, 2p) = \frac{768(70)^{1/2} \gamma_1^{3/2} \gamma_2^{5/2}}{(3)^{1/2} (\gamma_1 + \gamma_2)^3} (\gamma_2 - \gamma_1)(\gamma_2 - 2\gamma_1)$$

$$I(7d, 2p) = \frac{768(15)^{1/2} \gamma_1^{3/2} \gamma_2^{5/2}}{(3)^{1/2} (\gamma_1 + \gamma_2)^3} (\gamma_2 - \gamma_1)^3 (3\gamma_2 - 7\gamma_1)$$

$$I(3d, 3p) = \frac{256(5)^{1/2} \gamma_1^{7/2} \gamma_2^{5/2}}{(\gamma_1 + \gamma_2)^3} (2\gamma_1 - 5\gamma_2)$$

$$I(4d, 3p) = \frac{128(10)^{1/2} \gamma_1^{7/2} \gamma_2^{5/2}}{(\gamma_1 + \gamma_2)^3} \left(-8\gamma_1^2 + 33\gamma_1\gamma_2 - 15\gamma_2^2 \right).$$

TABLE B-5 (cont.)

$$I_{,}(5d,3p) = \frac{256(7)^{1/2} \gamma_1^{7/2} \gamma_2^{5/2}}{(\gamma_1 + \gamma_2)^{10}} \left[10\gamma_1^3 - 59\gamma_1^2 \gamma_2 + 60\gamma_1 \gamma_2^2 - 15\gamma_2^3 \right]$$

$$I_{,}(6d,3p) = \frac{512(35)^{1/2} \gamma_1^{7/2} \gamma_2^{5/2}}{(\gamma_1 + \gamma_2)^{11}} (\gamma_2 - \gamma_1) \left[4\gamma_1^3 - 27\gamma_1^2 \gamma_2 + 14\gamma_1 \gamma_2^2 - 5\gamma_2^3 \right]$$

$$I_{,}(7d,3p) = \frac{256(30)^{1/2} \gamma_1^{7/2} \gamma_2^{5/2}}{(\gamma_1 + \gamma_2)^{12}} (\gamma_2 - \gamma_1)^2 \left[14\gamma_1^3 - 107\gamma_1^2 \gamma_2 + 84\gamma_1 \gamma_2^2 - 15\gamma_2^3 \right]$$

$$I_{,}(6d,4p) = \frac{1280(42)^{1/2} \gamma_1^{7/2} \gamma_2^{5/2}}{(\gamma_1 + \gamma_2)^{12}} \left[\begin{aligned} & (\gamma_2 + \gamma_1)^5 - 7(\gamma_2 + \gamma_1)(\gamma_2 + \gamma_1)^4 \\ & + \frac{8}{5}(7\gamma_2^5 + 35\gamma_2^4 \gamma_1 + 10\gamma_2^3)(\gamma_2 + \gamma_1)^3 \\ & - \frac{12}{5}(42\gamma_2^2 \gamma_1 + 60\gamma_2 \gamma_1^2 + 5\gamma_1^3)(\gamma_2 + \gamma_1)^2 \\ & + 24(12\gamma_2^2 \gamma_1^2 + 5\gamma_2 \gamma_1^3)(\gamma_2 + \gamma_1) \\ & - 264\gamma_2^2 \gamma_1^3 \end{aligned} \right]$$

TABLE B-5 (cont.)

$$I(3d, 5p) = \frac{512(15)^{1/2} \delta^{1/2} \delta_1^{5/2}}{(\delta_1 + \delta_2)^9} \left[(\delta_1 + \delta_2)^3 - \frac{21}{2} (\delta_1 + \delta_2)^2 + \frac{168}{2} \delta_2 (\delta_1 + \delta_2) - \frac{1344}{625} \delta_2^3 \right]$$

$$I(6d, 5p) = \frac{1024(105)^{1/2} \delta^{1/2} \delta_1^{5/2}}{(\delta_1 + \delta_2)^9} \left[(\delta_1 + \delta_2)^5 - \frac{7}{2} (3\delta_1^2 + 2\delta_1) (\delta_1 + \delta_2)^5 \right. \\ \left. + \frac{1}{3} (42\delta_1^2 + 105\delta_1\delta_2 + 20\delta_2^2) (\delta_1 + \delta_2)^5 \right. \\ \left. - \frac{12}{5} (14\delta_1^3 + 126\delta_1^2\delta_2 + 90\delta_1\delta_2^2 + 5\delta_2^3) (\delta_1 + \delta_2)^3 \right. \\ \left. + 12 (28\delta_1^3\delta_2 + 72\delta_1^2\delta_2^2 + 15\delta_1\delta_2^3) (\delta_1 + \delta_2)^3 \right. \\ \left. - 264 (4\delta_1^3\delta_2^2 + 3\delta_1^2\delta_2^3) (\delta_1 + \delta_2) + 1056 \delta_1^3\delta_2^3 \right]$$

$$I(4d, 6p) = \frac{260(7)^{1/2} \delta_1^{1/2} \delta_2^{5/2}}{(\delta_1 + \delta_2)^9} \left[(\delta_1 + \delta_2)^5 - \frac{7}{3} (\delta_1 + 6\delta_2) (\delta_1 + \delta_2)^3 + \frac{112}{15} (5\delta_1\delta_2 + 2\delta_2^2) (\delta_1 + \delta_2)^3 \right. \\ \left. - \frac{232}{3} (3\delta_1\delta_2^2 + 2\delta_2^3) (\delta_1 + \delta_2)^3 + 32 (14\delta_1^3 + 3\delta_1^2\delta_2) (\delta_1 + \delta_2) \right. \\ \left. - 352 \delta_1^3 \delta_2^3 \right]$$

TABLE B-5 (cont.)

$$I_{,}(5d,6p) = \frac{2688(10)^{12} \beta_1^{12} \beta_2^{12}}{(\beta_1 + \beta_2)^{13}} \left[(\beta_1 + \beta_2)^5 - \frac{1}{5} (\beta_1 + \beta_2) (\beta_1 + \beta_2)^5 \right. \\ \left. + \frac{16}{15} (5\beta_1^2 + 10\beta_1\beta_2 + 6\beta_2\beta_1^2) (\beta_1 + \beta_2)^4 \right. \\ \left. - \frac{24}{5} (5\beta_1^2 + 21\beta_1\beta_2 + 7\beta_2\beta_1^2) (\beta_1 + \beta_2)^3 \right. \\ \left. + 32 (10\beta_1^2\beta_2^2 + 20\beta_1\beta_2^3 + 3\beta_2\beta_1^4) (\beta_1 + \beta_2)^2 \right. \\ \left. - 704 (2\beta_1^2\beta_2^2 + 3\beta_1\beta_2^3) (\beta_1 + \beta_2) + \frac{8416}{7} \beta_1^2\beta_2^4 \right]$$

$$I_{,}(4f,3d) = \frac{512(70)^{12} \beta_1^{12} \beta_2^{12}}{5(\beta_1 + \beta_2)^9} (\beta_2 - \beta_1)^4 (4\beta_1 - 4\beta_2)$$

$$I_{,}(5f,3d) = \frac{4096(7)^{12} \beta_1^{12} \beta_2^{12}}{5(\beta_1 + \beta_2)^9} (5\beta_1 - 4\beta_2)$$

$$I_{,}(6f,3d) = \frac{2048(105)^{12} \beta_1^{12} \beta_2^{12}}{5(\beta_1 + \beta_2)^9} (\beta_2 - \beta_1) (6\beta_1 - 4\beta_2)$$

TABLE B-5 (cont.)

$$I(7f,3d) = \frac{4096(3)^{1/2} \gamma_1^{3/2} \gamma_2^{1/2}}{(3_1+3_2)^{10}} (3_1-3_2)(7_3-4_3)$$

$$I(4f,4d) = \frac{1536(7)^{1/2} \gamma_1^{3/2} \gamma_2^{1/2}}{(3_1+3_2)^{10}} (3_1-2_3 \gamma_2)$$

$$I(5f,4d) = \frac{3072(70)^{1/2} \gamma_1^{3/2} \gamma_2^{1/2}}{5(3_1+3_2)^{10}} \left[-5 \gamma_1^2 + 17 \gamma_1 \gamma_2 - 8 \gamma_2^2 \right]$$

$$I(6f,4d) = \frac{1024(42)^{1/2} \gamma_1^{3/2} \gamma_2^{1/2}}{(3_1+3_2)^{10}} \left[9 \gamma_1^3 - 44 \gamma_1^2 \gamma_2 + 15 \gamma_1 \gamma_2^2 - 12 \gamma_2^3 \right]$$

$$I(7f,4d) = \frac{3072(30)^{1/2} \gamma_1^{3/2} \gamma_2^{1/2}}{(3_1+3_2)^{10}} (3_2-3_1)$$

$$\cdot \left[7 \gamma_1^3 - 38 \gamma_1^2 \gamma_2 + 35 \gamma_1 \gamma_2^2 - 8 \gamma_2^3 \right]$$

TABLE B-5 (cont.)

$$I(5f, 5d) = \frac{172032 \cdot 3^4 \cdot 3^4}{5(3_1 + 3_2)^2} \left[(3_2 + 3_1)^3 - \frac{6}{5} (53_2 + 33_1)(3_2 + 3_1)^5 + \frac{15}{7} (43_2^2 + 73_2 3_1)(3_2 + 3_1) - \frac{145}{7} 3_2^2 3_1 \right]$$

$$I(6f, 5d) = \frac{8016(15)^4 \cdot 3^4 \cdot 3^4}{5(3_1 + 3_2)^3} \left[(3_2 + 3_1)^4 - (33_2 + 3_1)(3_2 + 3_1)^3 + \frac{22}{63} (273_2^2 + 633_2 3_1 + 73_1^2)(3_2 + 3_1)^2 - \frac{220}{63} (273_2^2 3_1 + 143_2 3_1^2)(3_2 + 3_1) + \frac{1760}{63} 3_2^2 3_1^2 \right]$$

$$I(6f, 6d) = \frac{57344(3)^4 \cdot 3^4 \cdot 3^4}{(3_1 + 3_2)^4} \left[(3_2 + 3_1)^5 - \frac{9}{2} (23_2 + 3_1)(3_2 + 3_1)^4 + \frac{9}{2} (363_2^2 + 633_2 3_1 + 73_1^2)(3_2 + 3_1)^3 - 55 (33_2^3 + 183_2^2 3_1 + 73_1^3)(3_2 + 3_1)^2 - \frac{330}{7} (33_2^2 3_1 + 43_2 3_1^2)(3_2 + 3_1) + \frac{1430}{7} 3_2^3 3_1^2 \right]$$

B.10 Results of Computations*

(a) The Normalization Factor, $Q_{n\ell}$

$Q_{n\ell}$ is defined by Equation (B-13)

$$Q_{n\ell} = \left[\frac{(n+\ell)!}{2n(n\ell-1)!} \right]^{1/2} \frac{1}{(2\ell+1)!} \quad (B-13)$$

The following recursion relations are useful in extending a table of $Q_{n\ell}$:

$$Q_{n\ell} = \left[\frac{(n+\ell)(n-\ell)}{2\ell(2\ell+1)} \right]^{1/2} Q_{n,\ell-1} \quad (B-91)$$

$$Q_{n\ell} = \left[\frac{n-1}{n} \frac{n+\ell+1}{n-\ell} \right]^{1/2} Q_{n-1,\ell} \quad (B-92)$$

$$Q_{n\ell} = \left[\frac{n-1}{n} \frac{(n+\ell)(n+\ell-1)}{2\ell(2\ell+1)} \right]^{1/2} Q_{n-1,\ell-1} \quad (B-93)$$

A few special cases of $Q_{n\ell}$ are given below:

$$Q_{n,0} = 2^{-1/2} \quad (B-94)$$

$$Q_{n,1} = \frac{1}{6} \left[\frac{n^2-1}{2} \right]^{1/2}$$

$$Q_{n,n-1} = (2n)!^{-1/2} \quad (B-95)$$

A simple procedure in calculating $Q_{n\ell}$ is to start with Q_{n0} which is always $2^{-1/2}$, and successively calculate Q_{n1} , Q_{n2} , using Equation (B-91) until one arrives at $Q_{n,n-1}$. Equation (B-95) can be used as a final check.

* The work performed for this section was sponsored by both this contract and Contract No. AF 33(600)-42637.

The values of Q_{nl} for n up to 9 and all allowed values of l were computed in the above manner, and subsequently machine computations were also performed. Table B-6 lists the Q_{nl} .

(b) The Coefficients d_{nl}^i

The d_{nl}^i 's are the coefficients occurring in the hypergeometric function ${}_1F_1\left(-(n-l-1), 2l+2; x\right)$. They are given by Equation (B-15).

$$d_{nl}^i = (-1)^i \frac{(n-l-1)!}{(n-l-1-i)!} \frac{(2l+1)!}{(2l+1+i)!} \frac{1}{i!} \quad (B-15)$$

For $i > n-l-1$, d_{nl}^i vanishes.

The following recursion relations are useful in extending the table of d_{nl}^i :

$$d_{nl}^i = - \frac{(n-l-i)}{(2l+1+i)} d_{nl}^{i-1} \quad (B-97)$$

$$d_{nl}^i = \frac{(n-l-i)2l(2l+1)}{(n-l)(2l+1)(2l+1+i)} d_{n,l-1}^i \quad (B-98)$$

$$d_{nl}^i = \frac{n-l-1}{n-l-1-i} d_{n-1,l}^i \quad (B-99)$$

$$d_{nl}^i = \frac{2l(2l+1)}{(2l+1)(2l+1+i)} d_{n-1,l-1}^i \quad (B-100)$$

A few special cases of d_{nl}^i are of interest

$$d_{nl}^0 = 1 \quad (B-101)$$

TABLE B-6

 $Q_{n,l}$

$$Q_{ns} = 2^{-1/2} \text{ for all } n$$

n, l	Q	n, l	Q
2p	.204124E+00	8p	.935414E+00
3p	.333333E+00	8d	.362284E+00
3d	.372678E-01	8f	.639708E-01
4p	.456435E+00	8g	.615559E-02
4d	.790569E-01	8h	.349470E-03
4f	.498012E-02	8i	.118540E-04
5p	.577350E+00	8k	.218620E-06
5d	.132288E+00	9p	.105409E+01
5f	.125988E-01	9d	.462481E+00
5g	.524950E-03	9f	.934353E-01
6p	.697216E+00	9g	.104625E-01
6d	.197203E+00	9h	.711765E-03
6f	.243975E-01	9i	.306068E-04
6g	.151540E-02	9k	.824468E-06
6h	.456911E-04	9l	.124977E-07
7p	.816496E+00		
7d	.273861E+00		
7f	.412393E-01		
7g	.329030E-02		
7h	.146537E-03		
7i	.338685E-05		

$$d_{nl}^1 = -\frac{n-l-1}{2(l+1)} \quad (B-102)$$

$$d_{n,0}^i = (-1)^i \binom{n-1}{i} \frac{1}{(1+i)!} \quad (B-103)$$

A table of d_{nl}^1 for values of n up to 5 was prepared using the above recursion relations and subsequently machine computations were performed for n up to 9. These are given in Table B-7.

(c) The Screening Parameters

Equations (B-56) define a system of simultaneous non-linear equations in which the right hand side is a function of all the screening parameters $\pi_1, \pi_2, \dots, \pi_n$ of a given problem. A Fortran program for use on digital computers has been developed for solving these equations. We work along an isoelectronic sequence. We use as our starting point the case when $Z \rightarrow \infty$. The screening parameters for this case can be computed easily with $x_{\alpha\beta}$ given by Equation (B-61). As an intermediate step we perform iterative calculations for $Z = Z_0 + 40$, where Z_0 is the lowest member of the isoelectronic sequence, using π_α 's for $Z = \infty$ case as our starting point. The iterations are carried until the relative difference between the results of two successive iteration is less than a prescribed quantity ϵ (for computations reported here $\epsilon = 0.0001$). The process is repeated successively for the cases $Z = Z_0 + 19, Z_0 + 18, \dots, Z_0$. The screening parameters, expressed as $s(\alpha) (= \frac{n_\alpha}{2} \pi_\alpha)$ are given in Tables B-8 to B-19.

TABLE B-7

 $d_{n,l}^i$

i = 1 2 3 4 5 6 7 8

n,l

2s	-.500000E+00						
3p	-.250000E+00						
4p	-.166667E+00						
5p	-.125000E+00						
6p	-.100000E+00						
7p	-.833333E-01						
8p	-.714286E-01						
9p	-.625000E-01						
3s	-.100000E+01						
4s	-.500000E+00						
5s	-.333333E+00						
6s	-.250000E+00						
7s	-.200000E+00						
8s	-.166667E+00						
9s	-.142857E+00						
4s	-.150000E+01						
5p	-.750000E+00						
6d	-.500000E+00						
7f	-.375000E+00						
8g	-.300000E+00						
9h	-.250000E+00						

(1) $d_{n,l}^0 = 1$ for all cases

(11) For 1s, 2p, 3d, 4f, 5g, 6h, 7i, 8k, 9l,
 $d_{n,l}^0$ is the only non-vanishing coefficient

TABLE B-7 (continued)

<i>n, l</i>	1 = 1	2	3	4	5	6	7	8
	d_{nl}^1							
5s	-.200000E+01	.100000E+01	-.166667E+00	.833333E-02				
6p	-.100000E+01	.300000E+00	-.333333E-01	.119048E-02				
7d	-.666667E+00	.142857E+00	-.119048E-01	.330688E-03				
8f	-.500000E+00	.833333E-01	-.555556E-02	.126263E-03				
9g	-.400000E+00	.545455E-01	-.303030E-02	.582751E-04				
6s	-.250000E+01	.166667E+01	-.416667E+00	.416667E-01	-.138889E-02			
7p	-.125000E+01	.500000E+00	-.833333E-01	.595238E-02	-.148810E-03			
8d	-.833333E+00	.238095E+00	-.297619E-01	.165344E-02	-.330688E-04			
9f	-.625000E+00	.138889E+00	-.138889E-01	.631313E-03	-.105219E-04			
7s	-.300000E+01	.250000E+01	-.833333E+00	.125000E+00	-.833333E-02	.198413E-03		
8p	-.150000E+01	.750000E+00	-.166667E+00	.178571E-01	-.892857E-03	.165344E-04		
9d	-.100000E+01	.357143E+00	-.595238E-01	.496032E-02	-.198413E-03	.300625E-05		
8s	-.350000E+01	.350000E+01	-.145833E+01	.291667E+00	-.291667E-01	.138889E-02	-.248016E-04	
9p	-.175000E+01	.105000E+01	-.291667E+00	.416667E-01	-.312500E-02	.115741E-03	-.165344E-05	
9s	-.400000E+01	.466667E+01	-.233333E+01	.583333E+00	-.777778E-01	.555556E-02	-.198413E-03	.275573E-05

TABLE B-8
SCREENING PARAMETERS
Be I Isoelectronic Sequence
Configuration: $1s^2 2s^2$
Term: 1S

Ion	$s(1s)$	$s(2s)$
Li ⁻	3.2761 E-1	1.7902 E+0
Be I	3.1861 E-1	1.8599 E+0
B II	3.1369 E-1	1.8917 E+0
C III	3.1184 E-1	1.9025 E+0
N IV	3.1164 E-1	1.9036 E+0
O V	3.1221 E-1	1.9006 E+0
F VI	3.1312 E-1	1.8961 E+0
Ne VII	3.1414 E-1	1.8912 E+0
Na VIII	3.1517 E-1	1.8863 E+0
Mg IX	3.1616 E-1	1.8817 E+0
Al X	3.1708 E-1	1.8775 E+0
Si XI	3.1794 E-1	1.8736 E+0
P XII	3.1873 E-1	1.8700 E+0
S XIII	3.1946 E-1	1.8668 E+0
Cl XIV	3.2013 E-1	1.8639 E+0
Ar XV	3.2074 E-1	1.8612 E+0
K XVI	3.2130 E-1	1.8587 E+0
Ca XVII	3.2182 E-1	1.8565 E+0
Sc XVIII	3.2230 E-1	1.8544 E+0
Ti XIX	3.2274 E-1	1.8525 E+0
Z = ∞	3.3353 E-1	1.8078 E+0

TABLE B-9
 SCREENING PARAMETERS
 BeI Isoelectronic Sequence
 Configuration: $1s^2 2s2p$
 Term: 1P

Ion	s(1s)	s(2s)	s(2p)
Li ⁺	3.1832 E-1	1.5178 E+0	3.0030 E+0
Be I	3.2321 E-1	2.1229 E+0	2.0640 E+0
B II	3.2444 E-1	2.1965 E+0	1.9749 E+0
C III	3.2590 E-1	2.2165 E+0	1.9390 E+0
N IV	3.2766 E-1	2.2186 E+0	1.9180 E+0
O V	3.2949 E-1	2.2138 E+0	1.9037 E+0
F VI	3.3126 E-1	2.2065 E+0	1.8932 E+0
Ne VII	3.3289 E-1	2.1987 E+0	1.8849 E+0
Na VIII	3.3437 E-1	2.1911 E+0	1.8783 E+0
Mg IX	3.3570 E-1	2.1840 E+0	1.8728 E+0
Al X	3.3690 E-1	2.1775 E+0	1.8682 E+0
Si XI	3.3797 E-1	2.1715 E+0	1.8642 E+0
P XII	3.3893 E-1	2.1662 E+0	1.8608 E+0
S XIII	3.3980 E-1	2.1614 E+0	1.8578 E+0
Cl XIV	3.4059 E-1	2.1570 E+0	1.8551 E+0
Ar XV	3.4130 E-1	2.1530 E+0	1.8528 E+0
K XVI	3.4195 E-1	2.1494 E+0	1.8507 E+0
Ca XVII	3.4254 E-1	2.1461 E+0	1.8488 E+0
Sc XVIII	3.4308 E-1	2.1430 E+0	1.8471 E+0
Ti XIX	3.4358 E-1	2.1402 E+0	1.8456 E+0
Z = ∞	3.5507 E-1	2.0773 E+0	1.8129 E+0

TABLE B-10
SCREENING PARAMETERS
Be I Isoelectronic Sequence
Configuration: 1s²2s 3p
Term: 1_P

Ion	s(1s)	s(2p)	s(3p)
Li ⁻	3.1396 E-1	1.9799 E+0	2.5502 E+0
Be I	3.1969 E-1	1.8484 E+0	2.7110 E+0
B II	3.2529 E-1	1.7602 E+0	2.7775 E+0
C III	3.2957 E-1	1.7074 E+0	2.7953 E+0
N IV	3.3280 E-1	1.6774 E+0	2.7864 E+0
O V	3.3527 E-1	1.6598 E+0	2.7677 E+0
F VI	3.3720 E-1	1.6490 E+0	2.7471 E+0
Ne VII	3.3876 E-1	1.6419 E+0	2.7276 E+0
Na VIII	3.4003 E-1	1.6370 E+0	2.7102 E+0
Mg IX	3.4110 E-1	1.6334 E+0	2.6950 E+0
Al X	3.4200 E-1	1.6307 E+0	2.6818 E+0
Si XI	3.4276 E-1	1.6285 E+0	2.6703 E+0
P XII	3.4343 E-1	1.6268 E+0	2.6603 E+0
S XIII	3.4401 E-1	1.6253 E+0	2.6514 E+0
Cl XIV	3.4453 E-1	1.6240 E+0	2.6437 E+0
Ar XV	3.4498 E-1	1.6230 E+0	2.6368 E+0
K XVI	3.4539 E-1	1.6221 E+0	2.6306 E+0
Ca XVII	3.4575 E-1	1.6212 E+0	2.6251 E+0
Sc XVIII	3.4609 E-1	1.6205 E+0	2.6201 E+0
Ti XIX	3.4639 E-1	1.6199 E+0	2.6156 E+0
Z = ∞	3.5261 E-1	1.6072 E+0	2.5266 E+0

TABLE B-11
 SCREENING PARAMETERS
 O I Isoelectronic Sequence
 Configuration: $1s^2 2s^2 2p^4$
 Term: 1S

Ion	s(1s)	s(2s)	s(2p)
N ⁻	3.3288 E-1	2.9181 E+0	3.6713 E+0
O I	3.4078 E-1	3.0238 E+0	3.5794 E+0
F II	3.4825 E-1	3.0779 E+0	3.5248 E+0
Ne III	3.5524 E-1	3.1080 E+0	3.4873 E+0
Na IV	3.6170 E-1	3.1253 E+0	3.4595 E+0
Mg V	3.6763 E-1	3.1354 E+0	3.4378 E+0
Al VI	3.7303 E-1	3.1411 E+0	3.4204 E+0
Si VII	3.7794 E-1	3.1442 E+0	3.4061 E+0
P VIII	3.8241 E-1	3.1455 E+0	3.3940 E+0
S IX	3.8648 E-1	3.1458 E+0	3.3837 E+0
Cl X	3.9019 E-1	3.1453 E+0	3.3748 E+0
Ar XI	3.9358 E-1	3.1445 E+0	3.3671 E+0
K XII	3.9668 E-1	3.1433 E+0	3.3602 E+0
Ca XIII	3.9953 E-1	3.1420 E+0	3.3541 E+0
Sc XIV	4.0216 E-1	3.1406 E+0	3.3487 E+0
Ti XV	4.0458 E-1	3.1392 E+0	3.3438 E+0
V XVI	4.0682 E-1	3.1377 E+0	3.3394 E+0
Cr XVII	4.0890 E-1	3.1362 E+0	3.3353 E+0
Mn XVIII	4.1083 E-1	3.1348 E+0	3.3316 E+0
Fe XIX	4.1263 E-1	3.1334 E+0	3.3283 E+0
Z = ∞	4.6176 E-1	3.0813 E+0	3.2504 E+0

TABLE B-12
SCREENING PARAMETERS
Ca I Isoelectronic Sequence
Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4s$
Term: $3D$

Ion	$s(1s)$	$s(2s)$	$s(2p)$	$s(3s)$	$s(3p)$	$s(3d)$	$s(4s)$
Ca I	4.3125 E-1	4.0149 E+0	4.2567 E+0	9.3134 E+0	1.0536 E+1	1.4449 E+1	1.3226 E+1
Sc II	4.3603 E-1	4.0209 E+0	4.2559 E+0	9.3996 E+0	1.0597 E+1	1.3268 E+1	1.3277 E+1
Tl III	4.4070 E-1	4.0256 E+0	4.2559 E+0	9.4399 E+0	1.0610 E+1	1.2780 E+1	1.3318 E+1
V IV	4.4508 E-1	4.0301 E+0	4.2566 E+0	9.4651 E+0	1.0608 E+1	1.2466 E+1	1.3368 E+1
Cr V	4.4924 E-1	4.0348 E+0	4.2580 E+0	9.4821 E+0	1.0599 E+1	1.2236 E+1	1.3420 E+1
Mn VI	4.5319 E-1	4.0398 E+0	4.2598 E+0	9.4935 E+0	1.0586 E+1	1.2056 E+1	1.3471 E+1
Fe VII	4.5694 E-1	4.0451 E+0	4.2622 E+0	9.5009 E+0	1.0570 E+1	1.1910 E+1	1.3518 E+1
Co VIII	4.6051 E-1	4.0506 E+0	4.2649 E+0	9.5054 E+0	1.0552 E+1	1.1788 E+1	1.3561 E+1
Ni IX	4.6390 E-1	4.0565 E+0	4.2679 E+0	9.5076 E+0	1.0533 E+1	1.1683 E+1	1.3599 E+1
Cu X	4.6712 E-1	4.0625 E+0	4.2711 E+0	9.5080 E+0	1.0513 E+1	1.1594 E+1	1.3633 E+1
Zn XI	4.7019 E-1	4.0686 E+0	4.2744 E+0	9.5070 E+0	1.0493 E+1	1.1515 E+1	1.3663 E+1
Ca XII	4.7312 E-1	4.0748 E+0	4.2779 E+0	9.5049 E+0	1.0474 E+1	1.1445 E+1	1.3688 E+1
Ca XIII	4.7591 E-1	4.0811 E+0	4.2814 E+0	9.5020 E+0	1.0454 E+1	1.1383 E+1	1.3709 E+1
As XIV	4.7857 E-1	4.0874 E+0	4.2849 E+0	9.4985 E+0	1.0435 E+1	1.1327 E+1	1.3727 E+1
Se XV	4.8111 E-1	4.0937 E+0	4.2884 E+0	9.4945 E+0	1.0416 E+1	1.1277 E+1	1.3742 E+1
Br XVI	4.8354 E-1	4.0999 E+0	4.2919 E+0	9.4902 E+0	1.0398 E+1	1.1231 E+1	1.3753 E+1
Kr XVII	4.8587 E-1	4.1060 E+0	4.2954 E+0	9.4856 E+0	1.0381 E+1	1.1189 E+1	1.3763 E+1
Rb XVIII	4.8809 E-1	4.1120 E+0	4.2987 E+0	9.4808 E+0	1.0364 E+1	1.1150 E+1	1.3770 E+1
Sr XIX	4.9022 E-1	4.1179 E+0	4.3021 E+0	9.4759 E+0	1.0348 E+1	1.1115 E+1	1.3774 E+1
Y XX	4.9227 E-1	4.1237 E+0	4.3053 E+0	9.4709 E+0	1.0332 E+1	1.1082 E+1	1.3778 E+1
$Z = \infty$	5.8324 E-1	4.4093 E+0	4.4629 E+0	9.1595 E+0	9.7128 E+0	1.0216 E+1	1.3077 E+1

TABLE B-13
SCANNING PARAMETERS
Ca I Isoelectronic Sequence
Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4s$
Term: $1D$

Ion	$a(1s)$	$a(2s)$	$a(2p)$	$a(3s)$	$a(3p)$	$a(3d)$	$a(4s)$
Ca I	4.3125 E-1	4.0149 E+0	4.2566 E+0	9.3109 E+0	1.0541 E+1	1.4350 E+1	1.3301 E+1
Sc II	4.2609 E-1	4.0209 E+0	4.2559 E+0	9.4016 E+0	1.0598 E+1	1.3253 E+1	1.3310 E+1
Ti III	4.4071 E-1	4.0257 E+0	4.2559 E+0	9.4418 E+0	1.0610 E+1	1.2769 E+1	1.3349 E+1
V IV	4.4509 E-1	4.0303 E+0	4.2566 E+0	9.4670 E+0	1.0609 E+1	1.2455 E+1	1.3399 E+1
Cr V	4.4925 E-1	4.0350 E+0	4.2580 E+0	9.4838 E+0	1.0600 E+1	1.2225 E+1	1.3451 E+1
Mn VI	4.5320 E-1	4.0400 E+0	4.2599 E+0	9.4952 E+0	1.0586 E+1	1.2046 E+1	1.3502 E+1
Fe VII	4.5695 E-1	4.0453 E+0	4.2622 E+0	9.5025 E+0	1.0570 E+1	1.1909 E+1	1.3550 E+1
Co VIII	4.6051 E-1	4.0509 E+0	4.2649 E+0	9.5069 E+0	1.0552 E+1	1.1773 E+1	1.3593 E+1
Ni IX	4.6390 E-1	4.0567 E+0	4.2679 E+0	9.5090 E+0	1.0533 E+1	1.1674 E+1	1.3632 E+1
Cu X	4.6713 E-1	4.0627 E+0	4.2711 E+0	9.5092 E+0	1.0513 E+1	1.1585 E+1	1.3666 E+1
Zn XI	4.7020 E-1	4.0688 E+0	4.2744 E+0	9.5082 E+0	1.0493 E+1	1.1506 E+1	1.3696 E+1
Ca XII	4.7312 E-1	4.0750 E+0	4.2779 E+0	9.5060 E+0	1.0474 E+1	1.1437 E+1	1.3721 E+1
Sc XIII	4.7591 E-1	4.0813 E+0	4.2814 E+0	9.5030 E+0	1.0454 E+1	1.1375 E+1	1.3743 E+1
Cr XIV	4.7857 E-1	4.0876 E+0	4.2849 E+0	9.4994 E+0	1.0435 E+1	1.1319 E+1	1.3761 E+1
Sc XV	4.8112 E-1	4.0938 E+0	4.2884 E+0	9.4953 E+0	1.0416 E+1	1.1269 E+1	1.3776 E+1
Br XVI	4.8355 E-1	4.1000 E+0	4.2919 E+0	9.4909 E+0	1.0398 E+1	1.1223 E+1	1.3783 E+1
Kr XVII	4.8587 E-1	4.1061 E+0	4.2954 E+0	9.4862 E+0	1.0381 E+1	1.1182 E+1	1.3793 E+1
Br XVIII	4.8810 E-1	4.1121 E+0	4.2988 E+0	9.4814 E+0	1.0364 E+1	1.1143 E+1	1.3805 E+1
Sr XIX	4.9023 E-1	4.1180 E+0	4.3021 E+0	9.4764 E+0	1.0348 E+1	1.1108 E+1	1.3810 E+1
Y XX	4.9227 E-1	4.1238 E+0	4.3053 E+0	9.4714 E+0	1.0332 E+1	1.1073 E+1	1.3813 E+1
$z = \infty$	5.8324 E-1	4.4093 E+0	4.4629 E+0	9.1595 E+0	9.7128 E+0	1.0212 E+1	1.3112 E+1

TABLE B-14
SCATTERING PARAMETERS
No I Isoelectronic Sequence
Configuration: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d¹⁰ 4s² 4p⁶ 4d⁵ 5s
Tens: 7s

Ion	s(1s)	s(2s)	s(2p)	s(3s)	s(3p)	s(3d)	s(4s)	s(4p)	s(5s)	s(5p)
He I	4.9046 E-1	4.4951 E+0	4.5336 E+0	1.3364 E+1	1.4247 E+1	1.5389 E+1	2.2305 E+1	2.4031 E+1	2.8877 E+1	3.3597 E+1
He II	4.9263 E-1	4.5204 E+0	4.5707 E+0	1.3419 E+1	1.4258 E+1	1.5366 E+1	2.2554 E+1	2.4139 E+1	2.8616 E+1	2.9994 E+1
He III	4.9440 E-1	4.5410 E+0	4.5852 E+0	1.3450 E+1	1.4261 E+1	1.5343 E+1	2.2601 E+1	2.4171 E+1	2.8404 E+1	2.9319 E+1
He IV	4.9612 E-1	4.5604 E+0	4.5994 E+0	1.3470 E+1	1.4260 E+1	1.5321 E+1	2.2625 E+1	2.4192 E+1	2.8232 E+1	2.9097 E+1
He V	4.9780 E-1	4.5789 E+0	4.6133 E+0	1.3485 E+1	1.4257 E+1	1.5299 E+1	2.2642 E+1	2.4208 E+1	2.8085 E+1	2.8976 E+1
He VI	4.9944 E-1	4.5969 E+0	4.6269 E+0	1.3496 E+1	1.4253 E+1	1.5278 E+1	2.2656 E+1	2.4222 E+1	2.7954 E+1	2.8905 E+1
He VII	5.0103 E-1	4.6143 E+0	4.6402 E+0	1.3506 E+1	1.4248 E+1	1.5258 E+1	2.2669 E+1	2.4232 E+1	2.7834 E+1	2.8865 E+1
He VIII	5.0259 E-1	4.6311 E+0	4.6532 E+0	1.3513 E+1	1.4243 E+1	1.5240 E+1	2.2680 E+1	2.4241 E+1	2.7722 E+1	2.8843 E+1
He IX	5.0412 E-1	4.6476 E+0	4.6658 E+0	1.3520 E+1	1.4238 E+1	1.5222 E+1	2.2692 E+1	2.4248 E+1	2.7616 E+1	2.8834 E+1
He X	5.0560 E-1	4.6635 E+0	4.6782 E+0	1.3526 E+1	1.4232 E+1	1.5205 E+1	2.2702 E+1	2.4253 E+1	2.7516 E+1	2.8835 E+1
He XI	5.0705 E-1	4.6791 E+0	4.6903 E+0	1.3532 E+1	1.4227 E+1	1.5189 E+1	2.2711 E+1	2.4256 E+1	2.7419 E+1	2.8841 E+1
He XII	5.0847 E-1	4.6942 E+0	4.7021 E+0	1.3537 E+1	1.4223 E+1	1.5175 E+1	2.2720 E+1	2.4258 E+1	2.7326 E+1	2.8852 E+1
He XIII	5.0986 E-1	4.7090 E+0	4.7137 E+0	1.3542 E+1	1.4218 E+1	1.5161 E+1	2.2728 E+1	2.4258 E+1	2.7237 E+1	2.8866 E+1
He XIV	5.1121 E-1	4.7234 E+0	4.7250 E+0	1.3547 E+1	1.4214 E+1	1.5148 E+1	2.2735 E+1	2.4257 E+1	2.7150 E+1	2.8882 E+1
He XV	5.1253 E-1	4.7375 E+0	4.7360 E+0	1.3551 E+1	1.4210 E+1	1.5135 E+1	2.2742 E+1	2.4255 E+1	2.7066 E+1	2.8899 E+1
He XVI	5.1382 E-1	4.7512 E+0	4.7467 E+0	1.3556 E+1	1.4207 E+1	1.5124 E+1	2.2747 E+1	2.4251 E+1	2.6985 E+1	2.8916 E+1
He XVII	5.1509 E-1	4.7645 E+0	4.7572 E+0	1.3561 E+1	1.4204 E+1	1.5113 E+1	2.2752 E+1	2.4246 E+1	2.6907 E+1	2.8934 E+1
He XVIII	5.1632 E-1	4.7776 E+0	4.7674 E+0	1.3566 E+1	1.4201 E+1	1.5103 E+1	2.2756 E+1	2.4240 E+1	2.6831 E+1	2.8952 E+1
He XIX	5.1753 E-1	4.7903 E+0	4.7774 E+0	1.3571 E+1	1.4199 E+1	1.5093 E+1	2.2759 E+1	2.4232 E+1	2.6758 E+1	2.8969 E+1
He XX	5.1871 E-1	4.8028 E+0	4.7872 E+0	1.3575 E+1	1.4196 E+1	1.5084 E+1	2.2762 E+1	2.4224 E+1	2.6687 E+1	2.8986 E+1
$z = \infty$	6.1470 E-1	5.6751 E+0	5.4557 E+0	1.4110 E+1	1.4281 E+1	1.4749 E+1	2.1856 E+1	2.2574 E+1	2.3520 E+1	2.7754 E+1

TABLE B-15
SCHEMATIC PARAMETERS
Nb I Isoelectronic Sequence
Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^4 5s (5d) 5p$
Term: 7_D

Term	$s(1s)$	$s(2s)$	$s(2p)$	$s(3s)$	$s(3p)$	$s(3d)$	$s(4s)$	$s(4p)$	$s(4d)$	$s(5s)$	$s(5p)$
Nb I	4.3033 E-1	4.3025 E+0	4.3596 E+0	1.3367 E+1	1.4241 E+1	1.5375 E+1	2.2351 E+1	2.3970 E+1	2.8543 E+1	3.0278 E+1	2.9912 E+1
Nb II	4.3039 E-1	4.3244 E+0	4.5745 E+0	1.3408 E+1	1.4249 E+1	1.5352 E+1	2.2436 E+1	2.4004 E+1	2.8290 E+1	2.9363 E+1	2.9449 E+1
Nb III	4.3448 E-1	4.5443 E+0	4.5890 E+0	1.3431 E+1	1.4250 E+1	1.5329 E+1	2.2461 E+1	2.4018 E+1	2.8097 E+1	2.9064 E+1	2.9306 E+1
Nb IV	4.3623 E-1	4.5632 E+0	4.6030 E+0	1.3447 E+1	1.4246 E+1	1.5306 E+1	2.2474 E+1	2.4027 E+1	2.7937 E+1	2.8905 E+1	2.9219 E+1
Nb V	4.3733 E-1	4.5915 E+0	4.6167 E+0	1.3459 E+1	1.4241 E+1	1.5285 E+1	2.2484 E+1	2.4034 E+1	2.7797 E+1	2.8810 E+1	2.9206 E+1
Nb VI	4.3939 E-1	4.5990 E+0	4.6301 E+0	1.3468 E+1	1.4235 E+1	1.5264 E+1	2.2492 E+1	2.4039 E+1	2.7670 E+1	2.8751 E+1	2.9193 E+1
Cs VII	5.0122 E-1	4.6161 E+0	4.6431 E+0	1.3475 E+1	1.4228 E+1	1.5244 E+1	2.2499 E+1	2.4043 E+1	2.7553 E+1	2.8716 E+1	2.9192 E+1
La VIII	5.0281 E-1	4.6326 E+0	4.6558 E+0	1.3481 E+1	1.4221 E+1	1.5226 E+1	2.2505 E+1	2.4046 E+1	2.7443 E+1	2.8697 E+1	2.9198 E+1
Sc IX	5.0436 E-1	4.6486 E+0	4.6682 E+0	1.3486 E+1	1.4213 E+1	1.5208 E+1	2.2512 E+1	2.4047 E+1	2.7338 E+1	2.8689 E+1	2.9209 E+1
Sc X	5.0587 E-1	4.6643 E+0	4.6802 E+0	1.3490 E+1	1.4206 E+1	1.5192 E+1	2.2518 E+1	2.4047 E+1	2.7238 E+1	2.8688 E+1	2.9222 E+1
Sc XI	5.0734 E-1	4.6795 E+0	4.6920 E+0	1.3493 E+1	1.4199 E+1	1.5176 E+1	2.2523 E+1	2.4046 E+1	2.7143 E+1	2.8693 E+1	2.9235 E+1
I XII	5.0879 E-1	4.6943 E+0	4.7035 E+0	1.3496 E+1	1.4192 E+1	1.5161 E+1	2.2528 E+1	2.4043 E+1	2.7050 E+1	2.8702 E+1	2.9249 E+1
La XIII	5.1020 E-1	4.7087 E+0	4.7147 E+0	1.3500 E+1	1.4186 E+1	1.5148 E+1	2.2533 E+1	2.4040 E+1	2.6961 E+1	2.8713 E+1	2.9253 E+1
Cs XIV	5.1157 E-1	4.7220 E+0	4.7257 E+0	1.3503 E+1	1.4180 E+1	1.5134 E+1	2.2537 E+1	2.4035 E+1	2.6875 E+1	2.8726 E+1	2.9275 E+1
Sc XV	5.1292 E-1	4.7345 E+0	4.7364 E+0	1.3506 E+1	1.4174 E+1	1.5122 E+1	2.2540 E+1	2.4029 E+1	2.6792 E+1	2.8739 E+1	2.9286 E+1
La XVI	5.1423 E-1	4.7499 E+0	4.7468 E+0	1.3509 E+1	1.4168 E+1	1.5110 E+1	2.2543 E+1	2.4022 E+1	2.6711 E+1	2.8754 E+1	2.9296 E+1
Cs XVII	5.1552 E-1	4.7630 E+0	4.7570 E+0	1.3512 E+1	1.4164 E+1	1.5099 E+1	2.2545 E+1	2.4014 E+1	2.6633 E+1	2.8768 E+1	2.9304 E+1
Sc XVIII	5.1677 E-1	4.7758 E+0	4.7670 E+0	1.3516 E+1	1.4159 E+1	1.5089 E+1	2.2546 E+1	2.4005 E+1	2.6558 E+1	2.8782 E+1	2.9311 E+1
La XIX	5.1800 E-1	4.7883 E+0	4.7767 E+0	1.3519 E+1	1.4155 E+1	1.5079 E+1	2.2547 E+1	2.3996 E+1	2.6485 E+1	2.8796 E+1	2.9315 E+1
Sc XX	5.1921 E-1	4.8005 E+0	4.7861 E+0	1.3522 E+1	1.4151 E+1	1.5069 E+1	2.2548 E+1	2.3985 E+1	2.6415 E+1	2.8809 E+1	2.9319 E+1
Z = 90	6.1593 E-1	5.6595 E+0	5.4421 E+0	1.4011 E+1	1.4180 E+1	1.4693 E+1	2.1674 E+1	2.2368 E+1	2.3310 E+1	2.7524 E+1	2.7109 E+1

TABLE B-16
SCREENING PARAMETERS

No I Isoelectronic Sequence
Configuration: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d¹⁰ 4s² 4p⁶ 4d⁶
Term: 5_D

Ion	s(1s)	s(2s)	s(2p)	s(3s)	s(3p)	s(3d)	s(4s)	s(4p)	s(4d)
He I	4.9025 E-1	4.4943 E+0	4.5531 E+0	1.3402 E+1	1.4269 E+1	1.5401 E+1	2.2502 E+1	2.4214 E+1	2.9395 E+1
He II	4.9205 E-1	4.5139 E+0	4.5677 E+0	1.3432 E+1	1.4280 E+1	1.5382 E+1	2.2589 E+1	2.4281 E+1	2.9019 E+1
Hu III	4.9382 E-1	4.5331 E+0	4.5821 E+0	1.3454 E+1	1.4284 E+1	1.5361 E+1	2.2647 E+1	2.4321 E+1	2.8769 E+1
Hu IV	4.9555 E-1	4.5519 E+0	4.5962 E+0	1.3470 E+1	1.4284 E+1	1.5339 E+1	2.2692 E+1	2.4349 E+1	2.8579 E+1
He V	4.9725 E-1	4.5704 E+0	4.6101 E+0	1.3484 E+1	1.4282 E+1	1.5318 E+1	2.2731 E+1	2.4371 E+1	2.8420 E+1
Ag VI	4.9890 E-1	4.5884 E+0	4.6236 E+0	1.3496 E+1	1.4279 E+1	1.5297 E+1	2.2765 E+1	2.4389 E+1	2.8283 E+1
Cd VII	5.0051 E-1	4.6061 E+0	4.6371 E+0	1.3507 E+1	1.4275 E+1	1.5277 E+1	2.2795 E+1	2.4404 E+1	2.8159 E+1
La VIII	5.0209 E-1	4.6234 E+0	4.6502 E+0	1.3516 E+1	1.4271 E+1	1.5258 E+1	2.2823 E+1	2.4417 E+1	2.8044 E+1
Sc IX	5.0363 E-1	4.6403 E+0	4.6630 E+0	1.3525 E+1	1.4266 E+1	1.5240 E+1	2.2849 E+1	2.4427 E+1	2.7937 E+1
Sb X	5.0513 E-1	4.6569 E+0	4.6756 E+0	1.3534 E+1	1.4262 E+1	1.5224 E+1	2.2873 E+1	2.4436 E+1	2.7835 E+1
Ts XI	5.0660 E-1	4.6731 E+0	4.6878 E+0	1.3542 E+1	1.4258 E+1	1.5208 E+1	2.2896 E+1	2.4442 E+1	2.7738 E+1
I XII	5.0803 E-1	4.6889 E+0	4.6998 E+0	1.3551 E+1	1.4254 E+1	1.5193 E+1	2.2916 E+1	2.4446 E+1	2.7644 E+1
La XIII	5.0943 E-1	4.7044 E+0	4.7115 E+0	1.3559 E+1	1.4251 E+1	1.5179 E+1	2.2935 E+1	2.4449 E+1	2.7554 E+1
Cs XIV	5.1080 E-1	4.7195 E+0	4.7230 E+0	1.3567 E+1	1.4248 E+1	1.5166 E+1	2.2953 E+1	2.4450 E+1	2.7467 E+1
Rs XV	5.1213 E-1	4.7343 E+0	4.7342 E+0	1.3575 E+1	1.4245 E+1	1.5153 E+1	2.2968 E+1	2.4450 E+1	2.7383 E+1
La XVI	5.1344 E-1	4.7488 E+0	4.7451 E+0	1.3583 E+1	1.4243 E+1	1.5142 E+1	2.2983 E+1	2.4448 E+1	2.7302 E+1
Cs XVII	5.1472 E-1	4.7629 E+0	4.7558 E+0	1.3592 E+1	1.4240 E+1	1.5131 E+1	2.2996 E+1	2.4445 E+1	2.7223 E+1
Pr XVIII	5.1596 E-1	4.7767 E+0	4.7662 E+0	1.3600 E+1	1.4239 E+1	1.5121 E+1	2.3008 E+1	2.4441 E+1	2.7147 E+1
Mg XIX	5.1718 E-1	4.7902 E+0	4.7764 E+0	1.3608 E+1	1.4237 E+1	1.5111 E+1	2.3018 E+1	2.4435 E+1	2.7073 E+1
Pr XX	5.1838 E-1	4.8034 E+0	4.7864 E+0	1.3616 E+1	1.4236 E+1	1.5103 E+1	2.3028 E+1	2.4429 E+1	2.7001 E+1
Z = 60	6.1439 E-1	5.7007 E+0	5.4707 E+0	1.4240 E+1	1.4383 E+1	1.4810 E+1	2.2148 E+1	2.2765 E+1	2.3766 E+1

TABLE B-17
SCREENING PARAMETERS
No I Isoelectronic Sequence
Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^5 (4s)^5p$
Term: 7_p

Ion	s (1s)	s (2s)	s (2p)	s (3s)	s (3p)	s (3d)	s (4s)	s (4p)	s (4d)	s (5p)
No I	4.9032 E-1	4.4961 E+0	4.5549 E-0	1.3378 E+1	1.4245 E+1	1.5388 E+1	2.2366 E+1	2.4035 E+1	2.8824 E+1	3.5643 E+1
Te II	4.9210 E-1	4.5171 E+0	4.5712 E-0	1.3414 E+1	1.4266 E+1	1.5367 E+1	2.2474 E+1	2.4159 E+1	2.8611 E+1	3.1138 E+1
Br III	4.9389 E-1	4.5363 E+0	4.5858 E-0	1.3435 E+1	1.4271 E+1	1.5345 E+1	2.2525 E+1	2.4189 E+1	2.8396 E+1	3.0607 E+1
Bi IV	4.9564 E-1	4.5550 E+0	4.5999 E-0	1.3450 E+1	1.4271 E+1	1.5323 E+1	2.2560 E+1	2.4206 E+1	2.8223 E+1	3.0413 E+1
Pd V	4.9735 E-1	4.5732 E+0	4.6137 E-0	1.3461 E+1	1.4268 E+1	1.5302 E+1	2.2590 E+1	2.4218 E+1	2.8077 E+1	3.0315 E+1
Ag VI	4.9903 E-1	4.5909 E+0	4.6272 E+0	1.3471 E+1	1.4263 E+1	1.5281 E+1	2.2616 E+1	2.4227 E+1	2.7946 E+1	3.0263 E+1
Cd VII	5.0067 E-1	4.6083 E+0	4.6403 E+0	1.3480 E+1	1.4258 E+1	1.5261 E+1	2.2639 E+1	2.4234 E+1	2.7827 E+1	3.0237 E+1
In VIII	5.0227 E-1	4.6253 E+0	4.6532 E-0	1.3487 E+1	1.4252 E+1	1.5243 E+1	2.2661 E+1	2.4240 E+1	2.7715 E+1	3.0227 E+1
Sn IX	5.0383 E-1	4.6419 E+0	4.6657 E-0	1.3495 E+1	1.4246 E+1	1.5225 E+1	2.2682 E+1	2.4243 E+1	2.7610 E+1	3.0227 E+1
Sb X	5.0536 E-1	4.6581 E+0	4.6780 E+0	1.3501 E+1	1.4240 E+1	1.5209 E+1	2.2700 E+1	2.4246 E+1	2.7510 E+1	3.0234 E+1
Te XI	5.0685 E-1	4.6740 E+0	4.6899 E-0	1.3508 E+1	1.4234 E+1	1.5193 E+1	2.2718 E+1	2.4246 E+1	2.7413 E+1	3.0243 E+1
I XII	5.0831 E-1	4.6895 E+0	4.7016 E+0	1.3515 E+1	1.4228 E+1	1.5178 E+1	2.2734 E+1	2.4246 E+1	2.7321 E+1	3.0256 E+1
Te XIII	5.0973 E-1	4.7046 E+0	4.7130 E+0	1.3521 E+1	1.4223 E+1	1.5165 E+1	2.2748 E+1	2.4244 E+1	2.7232 E+1	3.0269 E+1
Cs XIV	5.1112 E-1	4.7195 E+0	4.7242 E+0	1.3528 E+1	1.4218 E+1	1.5152 E+1	2.2762 E+1	2.4240 E+1	2.7145 E+1	3.0282 E+1
Bi XV	5.1248 E-1	4.7340 E+0	4.7351 E+0	1.3534 E+1	1.4213 E+1	1.5139 E+1	2.2774 E+1	2.4236 E+1	2.7062 E+1	3.0294 E+1
La XVI	5.1381 E-1	4.7481 E+0	4.7457 E+0	1.3541 E+1	1.4209 E+1	1.5128 E+1	2.2785 E+1	2.4230 E+1	2.6981 E+1	3.0306 E+1
Cs XVII	5.1511 E-1	4.7619 E+0	4.7561 E+0	1.3547 E+1	1.4205 E+1	1.5117 E+1	2.2795 E+1	2.4223 E+1	2.6903 E+1	3.0317 E+1
Pr XVIII	5.1638 E-1	4.7755 E+0	4.7662 E+0	1.3554 E+1	1.4201 E+1	1.5107 E+1	2.2804 E+1	2.4216 E+1	2.6827 E+1	3.0326 E+1
Nd XIX	5.1762 E-1	4.7887 E+0	4.7761 E+0	1.3561 E+1	1.4198 E+1	1.5097 E+1	2.2811 E+1	2.4207 E+1	2.6754 E+1	3.0334 E+1
Pr XX	5.1883 E-1	4.8016 E+0	4.7858 E+0	1.3568 E+1	1.4195 E+1	1.5088 E+1	2.2818 E+1	2.4198 E+1	2.6684 E+1	3.0340 E+1
Z = ∞	6.1557 E-1	4.66853 E+0	5.4570 E+0	4.66853 E+0	1.4142 E+1	1.4754 E+1	2.1966 E+1	2.2558 E+1	2.3523 E+1	2.8047 E+1

TABLE P-18
SCHEFFING PARAMETERS
Cd I Isoelectronic Sequence
Configuration: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d¹⁰ 4s² 4p⁶ 4d¹⁰ 5s 5p
Term: 3_P

Ion	s (1s)	s (2s)	s (2p)	s (3s)	s (3p)	s (3d)	s (4s)	s (4p)	s (4d)	s (5s)	s (5p)
Cd I	5.0037 E-1	4.6058 E-0	4.6357 E+0	1.3687 E+1	1.4461 E+1	1.5412 E+1	2.3698 E+1	2.5493 E+1	3.0048 E+1	3.6007 E+1	3.4894 E+1
La II	5.0193 E-1	4.6289 E-0	4.6504 E+0	1.3742 E+1	1.4480 E+1	1.5480 E+1	2.3928 E+1	2.5590 E+1	2.9934 E+1	3.3496 E+1	3.3297 E+1
La III	5.0344 E-1	4.6487 E-0	4.6644 E+0	1.3774 E+1	1.4499 E+1	1.5388 E+1	2.4001 E+1	2.5624 E+1	2.9814 E+1	3.2875 E+1	3.2989 E+1
La IV	5.0490 E-1	4.6675 E-0	4.6781 E+0	1.3797 E+1	1.4495 E+1	1.5376 E+1	2.4045 E+1	2.5646 E+1	2.9703 E+1	3.2591 E+1	3.2854 E+1
La V	5.0632 E-1	4.6855 E-0	4.6915 E+0	1.3817 E+1	1.4499 E+1	1.5364 E+1	2.4077 E+1	2.5663 E+1	2.9600 E+1	3.2424 E+1	3.2782 E+1
La VI	5.0771 E-1	4.7031 E-0	4.7067 E+0	1.3834 E+1	1.4502 E+1	1.5353 E+1	2.4103 E+1	2.5676 E+1	2.9503 E+1	3.2318 E+1	3.2742 E+1
La VII	5.0907 E-1	4.7202 E-0	4.7176 E+0	1.3849 E+1	1.4504 E+1	1.5343 E+1	2.4125 E+1	2.5687 E+1	2.9410 E+1	3.2249 E+1	3.2723 E+1
La VIII	5.1040 E-1	4.7369 E-0	4.7303 E+0	1.3863 E+1	1.4507 E+1	1.5333 E+1	2.4145 E+1	2.5696 E+1	2.9321 E+1	3.2204 E+1	3.2715 E+1
La IX	5.1171 E-1	4.7532 E-0	4.7427 E+0	1.3877 E+1	1.4509 E+1	1.5324 E+1	2.4163 E+1	2.5703 E+1	2.9235 E+1	3.2176 E+1	3.2716 E+1
La X	5.1298 E-1	4.7690 E-0	4.7549 E+0	1.3889 E+1	1.4512 E+1	1.5316 E+1	2.4177 E+1	2.5708 E+1	2.9153 E+1	3.2160 E+1	3.2722 E+1
La XI	5.1423 E-1	4.7845 E-0	4.7668 E+0	1.3901 E+1	1.4514 E+1	1.5308 E+1	2.4194 E+1	2.5712 E+1	2.9073 E+1	3.2152 E+1	3.2731 E+1
La XII	5.1545 E-1	4.7996 E-0	4.7785 E+0	1.3913 E+1	1.4517 E+1	1.5301 E+1	2.4206 E+1	2.5714 E+1	2.8995 E+1	3.2150 E+1	3.2742 E+1
La XIII	5.1664 E-1	4.8144 E-0	4.7899 E+0	1.3924 E+1	1.4519 E+1	1.5294 E+1	2.4220 E+1	2.5715 E+1	2.8920 E+1	3.2153 E+1	3.2754 E+1
La XIV	5.1781 E-1	4.8288 E-0	4.8011 E+0	1.3935 E+1	1.4522 E+1	1.5288 E+1	2.4232 E+1	2.5715 E+1	2.8847 E+1	3.2160 E+1	3.2766 E+1
La XV	5.1896 E-1	4.8429 E-0	4.8120 E+0	1.3946 E+1	1.4525 E+1	1.5282 E+1	2.4242 E+1	2.5713 E+1	2.8776 E+1	3.2169 E+1	3.2778 E+1
La XVI	5.2009 E-1	4.8567 E-0	4.8227 E+0	1.3957 E+1	1.4528 E+1	1.5277 E+1	2.4251 E+1	2.5710 E+1	2.8708 E+1	3.2179 E+1	3.2790 E+1
La XVII	5.2118 E-1	4.8701 E-0	4.8331 E+0	1.3967 E+1	1.4532 E+1	1.5273 E+1	2.4260 E+1	2.5707 E+1	2.8641 E+1	3.2191 E+1	3.2801 E+1
La XVIII	5.2226 E-1	4.8833 E-0	4.8434 E+0	1.3978 E+1	1.4535 E+1	1.5269 E+1	2.4267 E+1	2.5702 E+1	2.8576 E+1	3.2203 E+1	3.2811 E+1
La XIX	5.2332 E-1	4.8961 E-0	4.8534 E+0	1.3988 E+1	1.4539 E+1	1.5265 E+1	2.4274 E+1	2.5697 E+1	2.8513 E+1	3.2216 E+1	3.2819 E+1
La XX	5.2435 E-1	4.9087 E-0	4.8632 E+0	1.3998 E+1	1.4543 E+1	1.5261 E+1	2.4280 E+1	2.5691 E+1	2.8452 E+1	3.2226 E+1	3.2826 E+1
$z = \infty$	6.1834 E-1	5.8502 E-0	5.5956 E+0	1.4908 E+1	1.5019 E+1	1.5284 E+1	2.3567 E+1	2.4158 E+1	2.5338 E+1	3.0615 E+1	3.0445 E+1

TABLE B-19

SCREENING PARAMETERS

Cd I Is-electronic Sequence
 Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^1$

Term: 1_p	$s(1s)$	$s(2s)$	$s(2p)$	$s(3s)$	$s(3p)$	$s(3d)$	$s(4s)$	$s(4p)$	$s(4d)$	$s(5s)$	$s(5p)$
Cd I	5.0032 E-1	4.6045 E+0	4.6357 E+0	1.3689 E+1	1.4465 E+1	1.5412 E+1	2.3684 E+1	2.5493 E+1	3.0034 E+1	3.7387 E+1	3.4010 E+1
La II	5.0190 E-1	4.6242 E+0	4.6499 E+0	1.3710 E+1	1.4474 E+1	1.5400 E+1	2.3757 E+1	2.5539 E+1	2.9904 E+1	3.6951 E+1	3.3343 E+1
La III	5.0347 E-1	4.6469 E+0	4.6641 E+0	1.3756 E+1	1.4486 E+1	1.5388 E+1	2.3955 E+1	2.5605 E+1	2.9805 E+1	3.4496 E+1	3.2712 E+1
La IV	5.0492 E-1	4.6669 E+0	4.6779 E+0	1.3791 E+1	1.4493 E+1	1.5376 E+1	2.4043 E+1	2.5640 E+1	2.9699 E+1	3.3328 E+1	3.2682 E+1
La V	5.0634 E-1	4.6853 E+0	4.6914 E+0	1.3814 E+1	1.4497 E+1	1.5364 E+1	2.4083 E+1	2.5660 E+1	2.9597 E+1	3.2921 E+1	3.2679 E+1
I VI	5.0773 E-1	4.7030 E+0	4.7046 E+0	1.3832 E+1	1.4501 E+1	1.5353 E+1	2.4111 E+1	2.5675 E+1	2.9500 E+1	3.2714 E+1	3.2675 E+1
La VII	5.0909 E-1	4.7202 E+0	4.7176 E+0	1.3848 E+1	1.4504 E+1	1.5343 E+1	2.4134 E+1	2.5687 E+1	2.9408 E+1	3.2592 E+1	3.2674 E+1
Cs VIII	5.1042 E-1	4.7369 E+0	4.7302 E+0	1.3863 E+1	1.4506 E+1	1.5333 E+1	2.4155 E+1	2.5696 E+1	2.9319 E+1	3.2516 E+1	3.2677 E+1
La IX	5.1172 E-1	4.7532 E+0	4.7427 E+0	1.3877 E+1	1.4509 E+1	1.5324 E+1	2.4173 E+1	2.5703 E+1	2.9233 E+1	3.2468 E+1	3.2683 E+1
La X	5.1299 E-1	4.7691 E+0	4.7548 E+0	1.3889 E+1	1.4511 E+1	1.5315 E+1	2.4189 E+1	2.5708 E+1	2.9151 E+1	3.2440 E+1	3.2691 E+1
Cs XI	5.1424 E-1	4.7847 E+0	4.7668 E+0	1.3902 E+1	1.4514 E+1	1.5307 E+1	2.4204 E+1	2.5712 E+1	2.9071 E+1	3.2426 E+1	3.2701 E+1
Pr XIII	5.1546 E-1	4.7998 E+0	4.7784 E+0	1.3913 E+1	1.4516 E+1	1.5300 E+1	2.4217 E-1	2.5714 E+1	2.8994 E+1	3.2420 E+1	3.2711 E+1
La XIII	5.1665 E-1	4.8146 E+0	4.7898 E+0	1.3925 E+1	1.4519 E+1	1.5294 E+1	2.4230 E+1	2.5715 E+1	2.8918 E+1	3.2442 E+1	3.2720 E+1
Pr XIV	5.1782 E-1	4.8290 E+0	4.8010 E+0	1.3936 E+1	1.4522 E+1	1.5288 E+1	2.4241 E+1	2.5715 E+1	2.8846 E+1	3.2428 E+1	3.2730 E+1
La XV	5.1897 E-1	4.8431 E+0	4.8119 E+0	1.3947 E+1	1.4525 E+1	1.5282 E+1	2.4251 E+1	2.5713 E+1	2.8775 E+1	3.2438 E+1	3.2738 E+1
La XVI	5.2009 E-1	4.8569 E+0	4.8226 E+0	1.3958 E+1	1.4528 E+1	1.5277 E+1	2.4260 E+1	2.5710 E+1	2.8706 E+1	3.2451 E+1	3.2746 E+1
Cs XVII	5.2119 E-1	4.8704 E+0	4.8331 E+0	1.3969 E+1	1.4532 E+1	1.5272 E+1	2.4269 E+1	2.5707 E+1	2.8639 E+1	3.2465 E+1	3.2752 E+1
Tb XVIII	5.2227 E-1	4.8835 E+0	4.8433 E+0	1.3979 E+1	1.4535 E+1	1.5268 E+1	2.4276 E+1	2.5702 E+1	2.8575 E+1	3.2480 E+1	3.2758 E+1
Dy XIX	5.2333 E-1	4.8964 E+0	4.8533 E+0	1.3990 E+1	1.4539 E+1	1.5265 E+1	2.4283 E+1	2.5697 E+1	2.8512 E+1	3.2497 E+1	3.2762 E+1
Ho XX	5.2436 E-1	4.9089 E+0	4.8631 E+0	1.4000 E+1	1.4543 E+1	1.5261 E+1	2.4288 E+1	2.5691 E+1	2.8451 E+1	3.2513 E+1	3.2764 E+1
Z = 69	6.1854 E-1	5.8502 E+0	5.5956 E+0	1.4908 E+1	1.5019 E+1	1.5284 E+1	2.3567 E+1	2.4158 E+1	2.5338 E+1	3.1201 E+1	3.0289 E+1

The hydrogenic wave functions using the screening parameters are compared with the self-consistent fieldwave functions for neutral oxygen (Hartree, Hartree and Swirles^(B-30)) and negative ion of lithium (Roothaan, Sachs, and Weiss^(B-31)) in Figures B-1 to B-4. The hydrogenic wave functions are given below:

O I ($1s^2 2s^2 2p^4 1S$) 1s electron: $42.394 r \exp(-7.6592 r)$

O I ($1s^2 2s^2 2p^4 1S$) 2s electron: $7.8491 r \exp(-2.4881r) (1-2.4881r)$

O I ($1s^2 2s^2 2p^4 1S$) 2p electron: $8.3864 r^2 \exp(-2.2103 r)$

Li ($1s^2 2s^2$) 2s electron: $0.94079 r \exp(-0.66524r) (1-0.66524r)$

The agreement between the two sets of wave functions is remarkable for O I and is good for Li.

Total ionization energies based on hydrogenic wave functions are compared with experimental values in Table B-20. The agreement is excellent; for Be I it is as good as that for the multiconfiguration Hartree-Fock wave functions of Kibartas, Kavetskis and Iutsis.^(B-32)

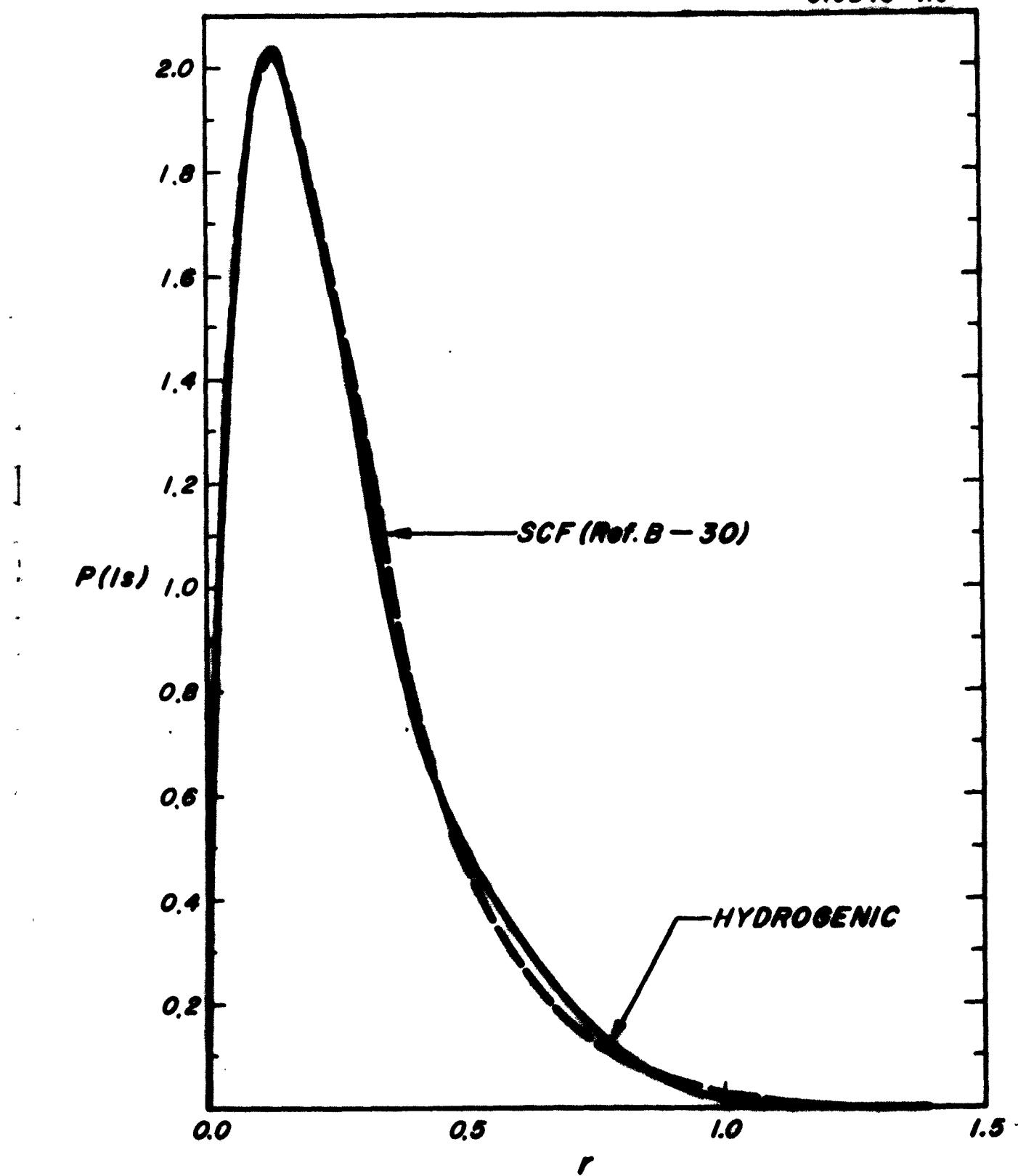


Figure B-1. OI ($1s^2 2s^2 2p^4 1s$): Wave Function of $1s$ Electron

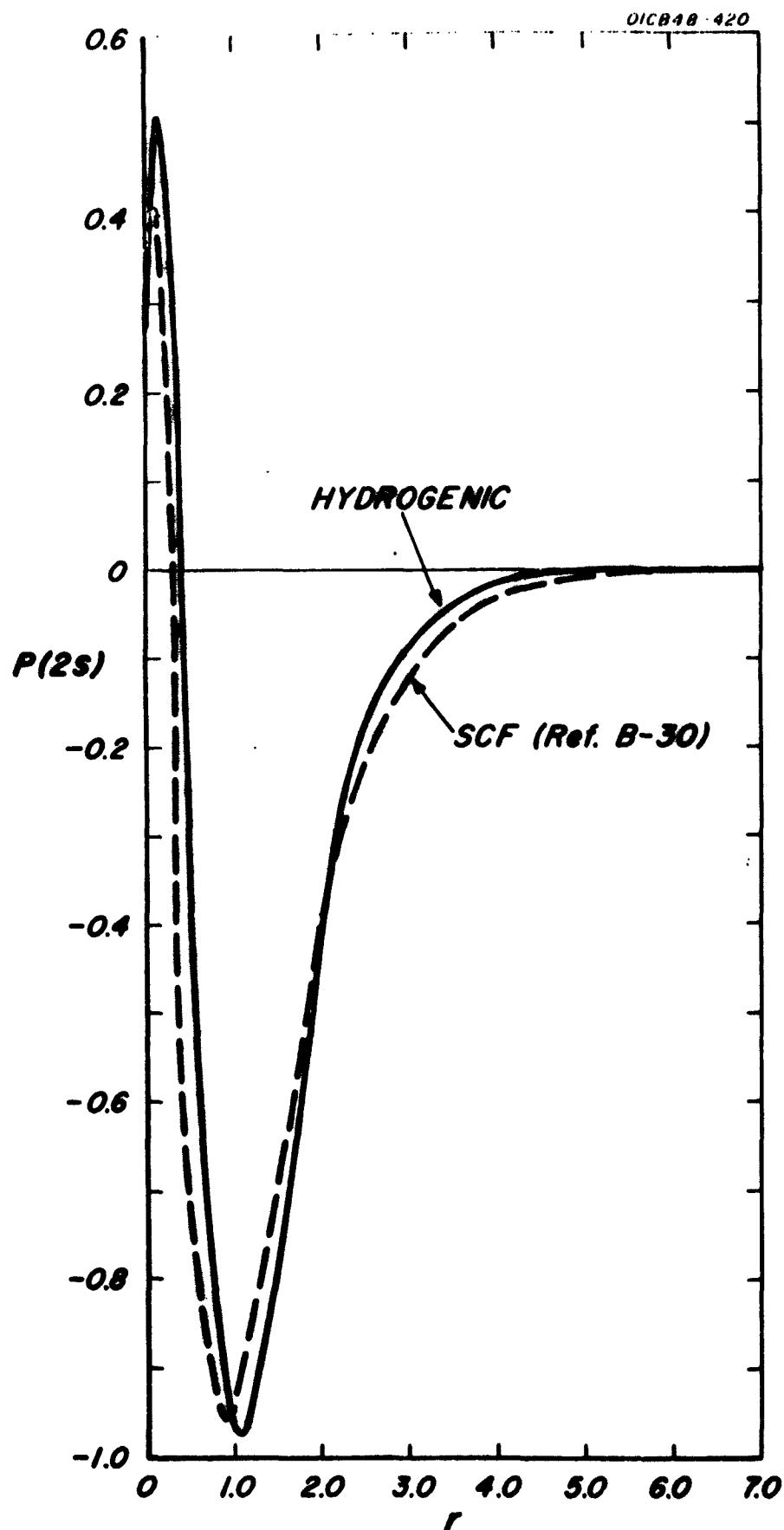


Figure B-2. OI ($1s^2 2s^2 2p^4 1s$): Wave Function of 2s Electron

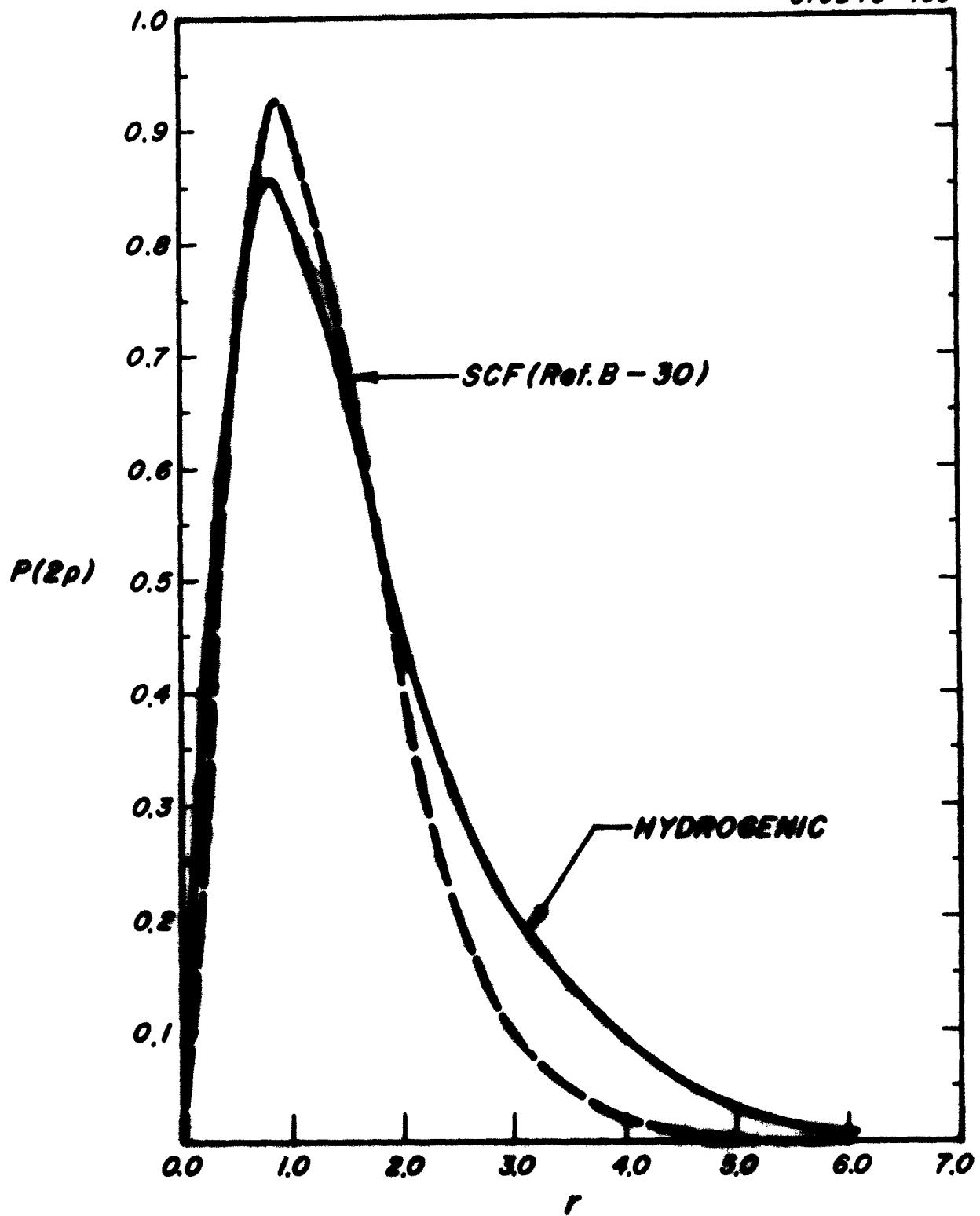


Figure B-3. OI ($1s^2 2s^2 2p^4 1s^1$): Wave Function of 2p Electron

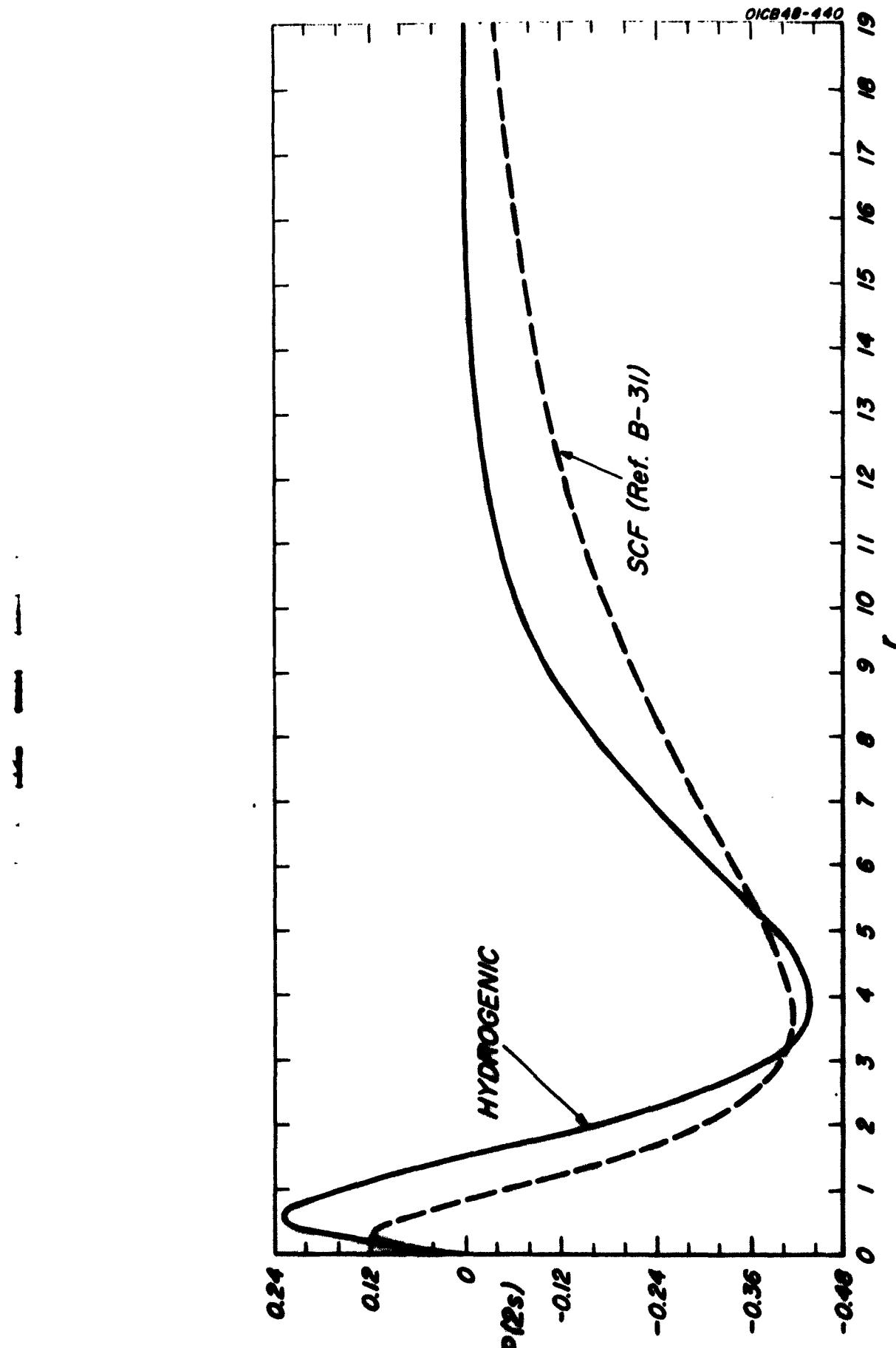


Figure 3-4. Li^- ($1s^2 2s^2$): Wave Function of 2s Electron

TABLE B-20
TOTAL IONIZATION ENERGIES (Atomic Unit)

	Hydrogenic Wave Function	H-F Wave Function	Experimental
O I (¹ S)	- 74.62		- 74.95
F II (¹ S)	- 98.61		- 98.92
Be I (¹ S)	- 14.70	- 14.64*	- 14.67
B II (¹ S)	- 24.38		- 24.35
C III (¹ S)	- 36.55		- 36.55
N IV (¹ S)	- 51.23		- 51.25
O V (¹ S)	- 68.40		- 68.45

*Based upon multiconfiguration Hartree-Fock calculations of Kibartas, Kavetskis and Iutsis. (B-32)

(d) The Dipole Integrals

The electric dipole integral I_1 is given by Equation (B-90) in terms of a coefficient $\gamma^u(n_1 l_1, n_2 l_2)$ defined by Equation (B-89). Computations on an IBM 7090 have been performed for the coefficients γ^u for all two-electron combinations of practical interest, and the results are given in Table B-21 to B-26. In order to reduce human errors in the reproduction of a large collection of numbers, the print-out from the digital computer has been photocopied. PSI 7, for example, means γ^7 . Numbers such as 0.23999999 or 0.24000011 should be rounded off to 0.24.

A few sample values of the transition integral σ^2 computed with the screened hydrogenic wave function are given in Table B-27, and compared with calculations based on Coulomb approximation (B-29) and H-F wave functions. The agreement is satisfactory.

TABLE B-21 Ψ^u (n_1, n_2, p)

<u><u>$n_1 = 1$</u></u>		<u><u>$n_2 = 2$</u></u>		<u><u>$n_1 = 3$</u></u>		<u><u>$n_2 = 4$</u></u>		<u><u>$n_1 = 1$</u></u>		<u><u>$n_2 = 5$</u></u>	
Ψ_1	0 = 0.23999999E 02	Ψ_1	0 = 0.26400000E 03	Ψ_1	0 = 0.263999999E 03	Ψ_1	0 = 0.263999999E 03	Ψ_1	0 = C.239999999E 02	Ψ_1	0 = C.239999999E 02
<u><u>$n_1 = 2$</u></u>	<u><u>$n_2 = 2$</u></u>	Ψ_1	1 = -0.17039999E 04	Ψ_1	1 = -0.24599999E 04	Ψ_1	1 = -0.24599999E 04	Ψ_1	1 = -C.14599999E 05	Ψ_1	1 = -C.14599999E 05
Ψ_1	0 = -0.95999999E 02	Ψ_1	2 = C.25679994E 04	Ψ_1	2 = C.64319994E 04	Ψ_1	2 = C.26799998E 05	Ψ_1	2 = -C.95999999E 02	Ψ_1	2 = -C.95999999E 02
Ψ_1	1 = C.23999999E 02	Ψ_1	3 = -0.19199998E 03	Ψ_1	3 = -0.56399998E 04	Ψ_1	3 = -C.23999999E 05	Ψ_1	3 = -C.10679999E 03	Ψ_1	3 = -C.10679999E 03
<u><u>$n_1 = 1$</u></u>	<u><u>$n_2 = 3$</u></u>	Ψ_1	4 = 0.48000000E 02	Ψ_1	4 = 0.12719999E 04	Ψ_1	4 = 0.14499994E 02	Ψ_1	4 = C.14499994E 02	Ψ_1	4 = C.14499994E 02
Ψ_1	0 = C.23999999E 02	Ψ_1	5 = -C.59999999E 02	Ψ_1	5 = -C.59999999E 02	Ψ_1	5 = -C.59999999E 02	Ψ_1	5 = -C.59999999E 02	Ψ_1	5 = -C.59999999E 02
<u><u>$n_1 = 2$</u></u>		<u><u>$n_2 = 3$</u></u>		<u><u>$n_1 = 4$</u></u>		<u><u>$n_2 = 5$</u></u>		<u><u>$n_1 = 4$</u></u>		<u><u>$n_2 = 6$</u></u>	
Ψ_1	0 = -C.95999999E 02	Ψ_1	0 = -C.57600000E 03	Ψ_1	0 = -0.57599996E 03	Ψ_1	0 = -0.57599996E 03	Ψ_1	0 = -C.95999999E 02	Ψ_1	0 = -C.95999999E 02
<u><u>$n_1 = 1$</u></u>	<u><u>$n_2 = 2$</u></u>	Ψ_1	1 = C.22299999E 03	Ψ_1	1 = 0.50599994E 04	Ψ_1	1 = C.71639998E 01	Ψ_1	1 = C.84000000E 03	Ψ_1	1 = C.84000000E 03
Ψ_1	2 = -C.36000000E 02	Ψ_1	2 = -C.10393999E 05	Ψ_1	3 = C.64320000E 04	Ψ_1	2 = -C.25451998E 05	Ψ_1	2 = -C.23039999E 04	Ψ_1	2 = -C.23039999E 04
<u><u>$n_1 = 3$</u></u>	<u><u>$n_2 = 3$</u></u>	Ψ_1	0 = 0.26399999E 03	Ψ_1	4 = -C.11519994E 04	Ψ_1	3 = C.32087999E 03	Ψ_1	3 = C.25453999E 04	Ψ_1	3 = C.25453999E 04
Ψ_1	1 = -C.94799999E 03	Ψ_1	5 = C.46000000F 02	Ψ_1	5 = C.16359999E 04	Ψ_1	4 = -C.15463999E 05	Ψ_1	4 = -C.10560000E 04	Ψ_1	4 = -C.10560000E 04
Ψ_1	2 = C.43200000E 03	Ψ_1	3 = -C.36000000E 02	Ψ_1	6 = -0.59999999E 02	Ψ_1	5 = 0.71999992E 02	Ψ_1	5 = 0.71999992E 02	Ψ_1	5 = 0.71999992E 02
<u><u>$n_1 = 1$</u></u>		<u><u>$n_2 = 2$</u></u>		<u><u>$n_1 = 5$</u></u>		<u><u>$n_2 = 5$</u></u>		<u><u>$n_1 = 5$</u></u>		<u><u>$n_2 = 6$</u></u>	
Ψ_1	0 = 0.23999999E 02	Ψ_1	1 = -0.10800000E 03	Ψ_1	0 = C.10799999E 04	Ψ_1	1 = -C.17049999E 05	Ψ_1	0 = C.26399999E 03	Ψ_1	0 = C.26399999E 03
<u><u>$n_1 = 1$</u></u>	<u><u>$n_2 = 2$</u></u>	Ψ_1	2 = C.72000000E 02	Ψ_1	3 = C.16399999E 03	Ψ_1	2 = 0.79343998E 05	Ψ_1	1 = -C.32159999E 04	Ψ_1	1 = -C.32159999E 04
Ψ_1	2 = C.47999997E 02	Ψ_1	3 = -C.59999999E 02	Ψ_1	4 = -C.95999998E 02	Ψ_1	3 = -C.13769199E 06	Ψ_1	2 = 0.12024000E 05	Ψ_1	2 = 0.12024000E 05
<u><u>$n_1 = 2$</u></u>	<u><u>$n_2 = 3$</u></u>	Ψ_1	0 = C.63600000E 03	Ψ_1	2 = -0.11879998E 04	Ψ_1	4 = C.92279992E 03	Ψ_1	3 = -0.17951999E 03	Ψ_1	3 = -0.17951999E 03
Ψ_1	1 = 0.43200000E 03	Ψ_1	3 = 0.70799995E 03	Ψ_1	4 = -C.23999999E 04	Ψ_1	5 = -0.24659998E 05	Ψ_1	4 = C.10679994E 03	Ψ_1	5 = -0.18719994E 04
Ψ_1	3 = C.87999997E 02	Ψ_1	4 = -C.59999999E 02	Ψ_1	7 = -C.59999999E 02	Ψ_1	6 = C.72000000E 02	Ψ_1	6 = C.72000000E 02	Ψ_1	6 = C.72000000E 02

TABLE B-21 $\Psi^u_{(n_1, n_2, p)}$ (continued)

<u>N1 = 6</u>		<u>N2 = 6</u>	
(6,6) (continued)		(3,7) (continued)	
PSI	7= C.70367990E 05	PSI	0=-C.18239999E 04
PSI	6= C.25919995E 04	PSI	0=-C.18239999E 04
PSI	8=-C.43199997E 04	PSI	1= 0.55557999E 04
PSI	2=-C.46019997E 05	PSI	2=-C.55122053E 05
PSI	9= C.72000000E 02	PSI	3= C.24295202E 07
N1 = 4	N2 = 6	N1 = 4	N2 = 6
PSI	0=-C.37600000E 05	PSI	4=-C.5280192E 07
PSI	1= C.11411999E 05	PSI	5= C.30464238E 07
PSI	2=-C.72027996E 05	PSI	6=-C.32636391E 07
PSI	1=-C.17999993E 05	PSI	7= C.90024010E 06
PSI	3= C.42605997E 05	PSI	8=-C.11544000E 05
PSI	4=-C.26688002E 04	PSI	9= C.39350999E 04
PSI	5= C.72000000E 02	PSI	10=-C.83344995E 02
N1 = 5	N2 = 6	N1 = 5	N2 = 7
PSI	0= C.10799999E 04	PSI	0= C.28566000E 04
PSI	1=-C.22031999E 05	PSI	1=-C.10236398E 04
PSI	2= 0.14011199E 06	PSI	2= C.12213602E 07
PSI	3=-0.36724798E 06	PSI	3=-C.63356210E 07
PSI	4= C.42247193E 06	PSI	4= C.16344400E 07
PSI	5=-C.21239999E 06	PSI	5=-C.25049734E 08
PSI	6= C.44592001E 05	PSI	6= 0.19018943E 08
N1 = 6	N2 = 6	N1 = 6	N2 = 7
PSI	0=-C.41199997E 01	PSI	0= C.28566000E 04
PSI	1=-C.46779993E 04	PSI	1=-C.10236398E 04
PSI	2= 0.14760000E 04	PSI	2= C.12213602E 07
PSI	3=-0.63999999E 02	PSI	3=-C.63356210E 07
PSI	4= 0.21030400E 06	PSI	4= C.16344400E 07
PSI	5=-C.772464C3E 06	PSI	5=-C.16673995E 06
PSI	6= C.13206238E 07	PSI	6= 0.70560019E 04
PSI	7=-C.35504002E 04	PSI	7=-C.77187569E 07
PSI	8= C.72000015E 02	PSI	8= C.16344400E 07
N1 = 6	N2 = 6	N1 = 3	N2 = 7
PSI	0= 0.26400000E 02	PSI	0= C.18239998E 04
PSI	1= 0.41159996E 05	PSI	1= 0.35839999E 05
PSI	2=-0.35769598E 06	PSI	2=-0.48240010E 04
PSI	3= C.11901119E 07	PSI	3=-0.83999992E 02
PSI	4=-C.18284078E 07	PSI	4= C.1100000E 05
PSI	5= 0.13206234E 07	PSI	5= 0.41159996E 05
PSI	6=-0.45254400E 06	PSI	6= 0.18204000E 05

TABLE 3-21 Ψ^u (a_1, a_2, p) (continued)

<u>$N1 = 1$</u>		<u>$N2 = 6$</u>		<u>$(6, 6)$ (continued)</u>	
p_{S1}	$0 = 0.23999999E\ 02$	p_{S1}	$0 = -0.57599997E\ 03$	p_{S1}	$2 = -C.76695987E\ 06$
p_{S1}	$1 = -C.21599999E\ 03$	p_{S1}	$1 = C.1336000E\ 05$	p_{S1}	$3 = C.43358402E\ 07$
p_{S1}	$2 = 0.71999993E\ 03$	p_{S1}	$2 = -C.10569599E\ 06$	p_{S1}	$4 = -C.12332150E\ 04$
p_{S1}	$3 = -0.12000000E\ 04$	p_{S1}	$3 = 0.37497595E\ 06$	p_{S1}	$5 = C.19018946E\ 08$
p_{S1}	$4 = C.10600000E\ 04$	p_{S1}	$4 = -0.67e61600E\ 06$	p_{S1}	$6 = -C.15995611E\ 08$
p_{S1}	$5 = -C.50399998E\ 03$	p_{S1}	$5 = C.64569587E\ 06$	p_{S1}	$7 = C.714720C5E\ 07$
p_{S1}	$6 = 0.96000122E\ 07$	p_{S1}	$6 = -C.30825666E\ 06$	p_{S1}	$8 = -C.163248C2E\ 07$
<u>$N1 = 2$</u>	<u>$N2 = 1$</u>	<u>$N1 = 5$</u>	<u>$N2 = 6$</u>	<u>$N1 = 7$</u>	<u>$N2 = 6$</u>
p_{S1}	$0 = -C.95999996E\ 02$	p_{S1}	$0 = -C.4875970E\ 04$	p_{S1}	$10 = -C.187399E04$
p_{S1}	$1 = C.12480000E\ 04$	p_{S1}	$1 = C.95399996E\ 02$	p_{S1}	$11 = C.95669996E\ 02$
p_{S1}	$2 = -0.56159996E\ 04$	p_{S1}	$2 = -C.10e60000E\ 04$	p_{S1}	$10 = -C.47d88599E\ 07$
p_{S1}	$3 = C.12600000E\ 07$	p_{S1}	$0 = C.10eCCCC0E\ 04$	p_{S1}	$11 = C.347327E1E\ 06$
p_{S1}	$4 = -C.13e39994E\ 02$	p_{S1}	$1 = -C.318e9997E\ 05$	p_{S1}	$12 = -C.10752C16E\ 05$
p_{S1}	$5 = 0.77760060E\ 04$	p_{S1}	$2 = C.313e4200E\ 04$	p_{S1}	$13 = C.956699936E\ 02$
p_{S1}	$6 = -C.19e79953E\ 04$	p_{S1}	$3 = -C.14e39996E\ 07$	p_{S1}	$1 = -C.12e6e794E\ 05$
p_{S1}	$7 = 0.9e000000E\ 02$	p_{S1}	$4 = C.32111919E\ 07$	p_{S1}	$2 = C.17339757E\ 07$
<u>$N1 = 3$</u>	<u>$N2 = 2$</u>	<u>$N1 = 5$</u>	<u>$N2 = 6$</u>	<u>$N1 = 7$</u>	<u>$N2 = 6$</u>
p_{S1}	$0 = 0.26399994E\ 03$	p_{S1}	$5 = -C.34163668E\ 07$	p_{S1}	$4 = C.3984e639E\ 05$
p_{S1}	$1 = -C.47279998E\ 04$	p_{S1}	$6 = 0.25047216E\ 07$	p_{S1}	$5 = -C.76305444E\ 04$
p_{S1}	$2 = C.283e1994E\ 05$	p_{S1}	$7 = -C.79152000E\ 06$	p_{S1}	$6 = C.622231708E\ 04$
p_{S1}	$3 = -0.78455999E\ 05$	p_{S1}	$8 = C.11339999E\ 06$	p_{S1}	$7 = -C.49661160E\ 04$
p_{S1}	$4 = 0.11148001E\ 06$	p_{S1}	$9 = -0.63600077E\ 04$	p_{S1}	$8 = 0.16550270E\ 06$
p_{S1}	$5 = -C.823e3976E\ 02$	p_{S1}	$10 = C.960000213E\ 02$	p_{S1}	$9 = -C.29314815E\ 07$
<u>$N1 = 6$</u>	<u>$N2 = 0$</u>			<u>$N1 = 1$</u>	<u>$N2 = 2$</u>
p_{S1}	$6 = 0.26728011E\ 05$	p_{S1}	$0 = 0.18240001E\ 04$	p_{S1}	$10 = C.25509606E\ 06$
p_{S1}	$7 = -0.34320000E\ 04$	p_{S1}	$11 = -0.92d79961E\ 04$	p_{S1}	$5 = -C.17639990E\ 04$
p_{S1}	$8 = C.923e3999E\ 02$	p_{S1}	$12 = 0.95444786E\ 02$	p_{S1}	$7 = -C.10799963E\ 05$

TABLE B-21 Ψ^u (n_1, s, n_2, p) (continued)

<u>$n_1 = 2$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 3$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 4$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 5$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 6$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 7$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 8$</u>		<u>$n_2 = 9$</u>	<u>$n_1 = 9$</u>	
PSI	0=-0.95999999E 02	PSI	6=-0.13051601E 07	PSI	7= C.533582393E 06	PSI	8=-0.14215193E 04	PSI	9= C.27538195E 07	PSI	10=-C.25808362E 06	PSI	11= C.99720078E 04	PSI	12=-C.28d49059E 07	PSI	13= C.1175d6608E 16	PSI	14=-C.11102126E 10	PSI	15=-C.11102126E 10	
PSI	1= C.14519999E 04	PSI	2=-C.78119995E 04	PSI	3= 0.20747998E 05	PSI	4=-C.30640000E 03	PSI	5= 0.25955991E 05	PSI	6=-0.12012000E 05	PSI	7= 0.25320049E 04	PSI	8=-C.10799963E 05	PSI	9= C.0.23371192E 07	PSI	10=-C.56416774E 07	PSI	11= C.79869040E 07	
PSI	2=-C.94631937E 05	PSI	3= 0.62520078E 04	PSI	4= 0.36821999E 03	PSI	5= 0.10800000E 04	PSI	6= 0.13921198E 06	PSI	7=-0.36821999E 03	PSI	8= C.28566000E 04	PSI	9= C.13692007E 03	PSI	10= C.1079975E 05	PSI	11= C.56416774E 07	PSI	12=-C.56416774E 07	
PSI	3= 0.25320049E 04	PSI	4= 0.25320049E 04	PSI	5= 0.36821999E 03	PSI	6= 0.10800000E 04	PSI	7= 0.13921198E 06	PSI	8= C.23371192E 07	PSI	9= C.18522935E 08	PSI	10= C.70074904E 06	PSI	11= C.59759843E 04	PSI	12=-C.56416049E 06	PSI	13= C.13692007E 03	
PSI	4= 0.26399999E 05	PSI	5= 0.54239998E 04	PSI	6= 0.10006075E 04	PSI	7= 0.66587035E 07	PSI	8= 0.123123159E 07	PSI	9= 0.23123159E 07	PSI	10= 0.36821999E 06	PSI	11= 0.42695995E 06	PSI	12= 0.46695995E 06	PSI	13= 0.5367420E 07	PSI	14=-C.49470229E 06	
PSI	5= 0.15339199E 06	PSI	6= 0.14418403E 06	PSI	7= 0.42167984E 05	PSI	8= 0.15339199E 06	PSI	9= 0.25734390E 06	PSI	10= 0.42167984E 05	PSI	11= 0.51291130E 07	PSI	12= 0.6136313E 10	PSI	13= 0.716436313E 10	PSI	14=-C.91461696E 06	PSI	15=-C.11604230E 04	
PSI	6= 0.13494947E 06	PSI	7= 0.14418403E 06	PSI	8= 0.16260406E 06	PSI	9= 0.18111992E 04	PSI	10= 0.13494947E 07	PSI	11= 0.16260406E 06	PSI	12= 0.18111992E 04	PSI	13= 0.194124099E 07	PSI	14= 0.23760412E 06	PSI	15= 0.3655700C 07	PSI	16= 0.49470229E 06	
PSI	7= 0.42167984E 05	PSI	8= 0.43426036E 04	PSI	9= 0.16799886E 03	PSI	10= 0.18240002E 04	PSI	11= 0.15337199E 05	PSI	12= 0.18240002E 04	PSI	13= 0.16799886E 03	PSI	14= 0.17534199E 05	PSI	15= 0.18240002E 04	PSI	16= 0.194124099E 07	PSI	17= 0.20325229E 06	
PSI	8= 0.13494947E 06	PSI	9= 0.14418403E 06	PSI	10= 0.16260406E 06	PSI	11= 0.18240002E 04	PSI	12= 0.15337199E 05	PSI	13= 0.16799886E 03	PSI	14= 0.17534199E 05	PSI	15= 0.18240002E 04	PSI	16= 0.194124099E 07	PSI	17= 0.20325229E 06	PSI	18= 0.21759651E 04	
PSI	9= 0.16799886E 03	PSI	10= 0.18240002E 04	PSI	11= 0.15337199E 05	PSI	12= 0.16799886E 03	PSI	13= 0.17534199E 05	PSI	14= 0.18240002E 04	PSI	15= 0.194124099E 07	PSI	16= 0.20325229E 06	PSI	17= 0.21759651E 04	PSI	18= 0.233522355E 04	PSI	19= 0.24995039E 07	

TABLE B-22 Ψ^u (n₁P, n₂s)

TABLE B-22 Ψ' ($n_1 P, n_2 s$) (continued)

<u>$n_1 = 6$</u>	<u>$n_2 = 7$</u>								
Ψ_1	0= 0.720000000E 02	Ψ_1	5= 0.24771601E 06	Ψ_1	5= 0.71999992E 02	Ψ_1	0= C.71999992E 02	Ψ_1	0= C.23999999E 02
Ψ_1	1=-0.513400000E 04	Ψ_1	6=-0.16657197E 06	Ψ_1	1=-0.59519990E 04	Ψ_1	1=-0.7674998E 03	Ψ_1	1=-0.51671997E 03
Ψ_1	2= 0.10202399E 06	Ψ_1	7= 0.51108000E 05	Ψ_1	2= C.13955999E 06	Ψ_1	2= C.73919997E 04	Ψ_1	2= C.75239986E 05
Ψ_1	3=-C.82866399E 06	Ψ_1	8=-0.42239970E 04	Ψ_1	3=-C.13720319E 07	Ψ_1	3=-0.32255999E 05	Ψ_1	3=-0.32255999E 05
Ψ_1	4= 0.32119197E 07	<u>$n_1 = 4$</u>	<u>$n_2 = 8$</u>	Ψ_1	4= C.66587029E 07	Ψ_1	4= C.75239986E 05	Ψ_1	4= C.75239986E 05
Ψ_1	5=-0.63368639E 07	Ψ_1	0= 0.48000000E 02	Ψ_1	5=-0.17265025E 08	Ψ_1	5=-0.10214402E 06	Ψ_1	5=-0.10214402E 06
Ψ_1	6= 0.64392467E 07	Ψ_1	1=-0.25919999E 04	Ψ_1	6= C.246666762E 08	Ψ_1	6= C.79467968E 07	Ψ_1	6= C.79467968E 07
Ψ_1	7=-0.32757117E 07	Ψ_1	2= 0.39167998E 05	Ψ_1	7=-C.19284481E 06	Ψ_1	7=-C.33792055E 05	Ψ_1	7=-C.33792055E 05
Ψ_1	8= 0.79427206E 06	Ψ_1	3=-C.246662399E 06	Ψ_1	8= C.79209360E 07	Ψ_1	8= C.59753805E 04	Ψ_1	8= C.59753805E 04
Ψ_1	9=-0.84239992E 05	Ψ_1	4= 0.76406390E 06	Ψ_1	9=-0.16110715E 07	Ψ_1	9=-0.16110715E 07	<u>$n_1 = 3$</u>	<u>$n_2 = 9$</u>
Ψ_1	10= C.28566C004E 04	Ψ_1	5=-0.12519360E 07	Ψ_1	10= C.14445603E 06	Ψ_1	10= C.-35999999E 02	Ψ_1	10= C.-35999999E 02
<u>$n_1 = 2$</u>	<u>$n_2 = 6$</u>	Ψ_1	6= C.10913280E 07	Ψ_1	11=-C.42239980E 04	Ψ_1	11= C.16559996E 04	Ψ_1	11= C.16559996E 04
Ψ_1	7=-C.47145600E 06	<u>$n_1 = 7$</u>	<u>$n_2 = 6$</u>	Ψ_1	7=-0.21935999E 05	Ψ_1	7=-0.21935999E 05	Ψ_1	7=-0.21935999E 05
Ψ_1	0= 0.23999999E 02	Ψ_1	8= 0.82223966E 05	Ψ_1	0=-C.84000061E 07	Ψ_1	3= C.12635599E 06	Ψ_1	3= C.12635599E 06
Ψ_1	1=-0.67199998E 03	Ψ_1	9=-0.42239951E 04	Ψ_1	1= C.-81720000E 04	Ψ_1	4=-C.37749595E 06	Ψ_1	4=-C.37749595E 06
Ψ_1	2= 0.55439997E 04	<u>$n_1 = 5$</u>	<u>$n_2 = 8$</u>	Ψ_1	2=-0.22748397E 06	Ψ_1	5= C.63337603E 06	Ψ_1	5= C.63337603E 06
Ψ_1	3=-0.20159999E 05	Ψ_1	0=-0.59999996E 02	Ψ_1	3= 0.267t8209E 07	Ψ_1	6=-0.61121594E 06	Ψ_1	6=-0.61121594E 06
Ψ_1	4= 0.37800000E 05	Ψ_1	1= 0.40920000E 04	Ψ_1	4=-C.15723725E 08	Ψ_1	7= C.32009593E 00	Ψ_1	7= C.32009593E 00
Ψ_1	5=-0.38304033E 05	Ψ_1	2=-0.78479999E 05	Ψ_1	5= C.49919536E 08	Ψ_1	8= C.83555999E 05	Ψ_1	8= C.83555999E 05
Ψ_1	6= 0.19991992E 05	Ψ_1	3= 0.62683190E 06	Ψ_1	6=-0.89022999E 08	Ψ_1	9= 0.59759882E 04	Ψ_1	9= 0.59759882E 04
Ψ_1	7=-0.42240009E 04	Ψ_1	4=-0.24570001E 07	Ψ_1	7= C.89886036E 08	<u>$n_1 = 4$</u>	<u>$n_2 = 7$</u>	Ψ_1	<u>$n_2 = 7$</u>
<u>$n_1 = 3$</u>	<u>$n_2 = 6$</u>	Ψ_1	5= C.51019922E 07	Ψ_1	8=-C.50673039E 08	Ψ_1	0= 0.48000030E 02	Ψ_1	2= 0.51671997E 03
Ψ_1	0=-0.35999999E 02	Ψ_1	6=-C.57324955E 07	Ψ_1	9= 0.15527586E 08	Ψ_1	1=-0.29519999E 04	Ψ_1	3=-0.38582399E 06
Ψ_1	1= 0.14519999E 04	Ψ_1	7= 0.33789602E 07	Ψ_1	10=-0.24458030E 07	Ψ_1	11= 0.17557199E 06	Ψ_1	12=-0.42239980E 04
Ψ_1	2=-0.16548000E 05	Ψ_1	8=-0.95295550E 06	Ψ_1	12= 0.14649598E 07	Ψ_1	13= 0.30868319E 07	Ψ_1	14=-0.30868319E 07

TABLE B-22 Ψ^u ($\eta_1 P, \eta_2 S$) (continued)

(4,9) (continued)		$N1= 6$		$N2= 9$		$N1= 7$		$N2= 9$		$N1= 8$		$N2= 9$	
PSI 6= 0.37299357E 07	PSI 0= 0.71999992E 02	PSI 0= -0.840000030E 02	PSI 0= -0.840000030E 02	PSI 1= -0.67660000E 04	PSI 1= C.92E6C009E 04	PSI 1= -0.12215996E 05	PSI 1= -0.12215996E 05	PSI 2= -0.29767197E 06	PSI 2= C.45361625E 06	PSI 3= -C.73049740E 07	PSI 3= -C.73049740E 07	PSI 4= C.60364623E 06	PSI 4= C.60364623E 06
PSI 8= 0.89755212E 06	PSI 2= 0.18297598E 06	PSI 3= -0.211127202E 07	PSI 3= 0.41031355E 07	PSI 4= -C.26606542E 06	PSI 4= -C.26606542E 06	PSI 5= C.11254299E 04	PSI 5= -C.2660101C8E 04	PSI 6= -C.25640734E 04	PSI 6= -C.25640734E 04	PSI 7= C.34715613E 03	PSI 7= -C.12668164E 10	PSI 8= C.76679072E 04	PSI 8= C.76679072E 04
PSI 9= -0.13331994E 06	PSI 4= C.12345474E 06	PSI 5= -C.39E73890E 08	PSI 5= -C.39E73890E 08	PSI 6= 0.74386363E 06	PSI 6= -C.25640734E 04	PSI 7= -0.81076088E 08	PSI 7= -0.81076088E 08	PSI 8= C.50659791E 08	PSI 8= -C.27E277C0E 09	PSI 9= -C.12907825E 09	PSI 9= -C.12907825E 09	PSI 10= -0.35395704E 08	PSI 10= -0.35395704E 08
PSI 10= 0.59759882E 04	PSI 1= C.46560000E 04	PSI 7= -0.81076088E 08	PSI 8= C.50659791E 08	PSI 9= -C.17271584E 06	PSI 9= -C.17271584E 06	PSI 10= 0.29940449E 07	PSI 10= 0.29940449E 07	PSI 11= C.45218860E 07	PSI 11= C.45218860E 07	PSI 12= -C.57572444E 06	PSI 12= -C.57572444E 06	PSI 13= C.59760000E 04	PSI 13= C.59760000E 04
PSI 5= C.12140351E 06	PSI 6= -0.18299732E 06	PSI 7= 0.15641868E 08	PSI 8= -C.75400434E 07	PSI 9= 0.17059360E 07	PSI 10= -0.18308387E 06	PSI 11= C.59759843E 04	PSI 12= C.59759843E 04	PSI 13= -C.332375C0E 06	PSI 14= C.54754922E 04	PSI 14= C.54754922E 04	PSI 14= C.54754922E 04	PSI 14= C.54754922E 04	PSI 14= C.54754922E 04

TABLE B-23 $\Psi^u_{(n_1 p, n_2 s)}$

<u>N1= 2</u>	<u>N2= 3</u>	<u>N1= 2</u>	<u>N2= 5</u>	<u>N1= 6</u>	<u>N2= 3</u>	<u>N1= 5</u>	<u>N2= 6</u>
PSI 0= 0.72000000E 03		PSI 0= 0.72000000E 03		PSI 0= C.11375999E 03		PSI 0= -0.68399999E 04	
N1= 3	N2= 3			PSI 1= -C.19199999E 04		PSI 1= C.70343997E 05	
PSI 0=-0.18000000E 04		PSI 2= 0.11999999E 04		PSI 2= 0.29442514E 06		PSI 2= -C.22708799E 06	
PSI 1= C.72000000E 03				PSI 3= -C.30278398E 06		PSI 3= 0.28699198E 06	
<u>N1= 4</u>	<u>N2= 3</u>	<u>N1= 3</u>	<u>N2= 5</u>	PSI 4= 0.15032000E 06		PSI 4= -C.14133600E 06	
PSI 0= C.37439999E 04		PSI 0= -C.18000000E 04		PSI 5= -C.22555999E 05		PSI 5= C.26219998E 05	
PSI 1=-0.36000000E 04		PSI 1= C.71999999E 04		PSI 6= C.11999999E 04		PSI 6= -C.14399999E 04	
PSI 2= 0.72000000E 03		PSI 2= -0.70799998E 04		N1= 2	N2= 6	N1= 6	N2= 6
N1= 2	N2= 4			PSI 0= C.71499999E 03		PSI 0= C.11375999E 05	
PSI 0= 0.72000000E 03		PSI 3= 0.11999999E 04		PSI 1= -C.286799999E 04		PSI 1= -C.14572800E 06	
PSI 1=-0.95999999E 03				PSI 2= C.36000000E 04		PSI 2= C.60189994E 06	
N1= 3	N2= 4	N1= 4	N2= 5	PSI 3= -C.14399999E 04		PSI 3= -C.10239222E 07	
PSI 0=-C.16000000E 04		PSI 0= 0.37440000E 04		N1= 3	N2= 6	PSI 4= C.17570740E 06	
PSI 1= 0.39599999E 04		PSI 1= -C.20475999E 05		PSI 0= -C.17499999E 04		PSI 5= -C.248832C0E 06	
PSI 2=-C.45399999E 03		PSI 2= C.30959999E 05		PSI 1= C.10439999E 05		PSI 6= C.35C39998E 05	
N1= 4	N2= 4			PSI 2= -C.18355999E 05		PSI 7= -C.14399960E 04	
PSI 0= C.37439999E 04		PSI 4= 0.12000000E 04		PSI 3= C.11160000E 05		N1= 7	N2= 6
PSI 1=-C.12287999E 05				PSI 4= -C.14399999E 04		PSI 0= -C.1764C0C1E 05	
PSI 2= C.71699999E 04				PSI 5= C.27252000E 06		PSI 1= C.27252000E 06	
PSI 3=-C.95449999E 03		N1= 5	N2= 5	N1= 4	N2= 6	PSI 2= -C.13913996E 07	
N1= 5	N2= 4			PSI 0= -0.68399999E 04		PSI 3= C.30527489E 07	
PSI 0=-C.68399999E 04		PSI 1= 0.50639997E 05		PSI 1= -C.29663999E 05		PSI 4= -C.31363707E 07	
PSI 1= C.30435999E 05		PSI 2= -0.10535999E 06		PSI 2= 0.71999995E 05		PSI 5= 0.158364C1E 07	
PSI 2=-0.31463999E 05		PSI 3= 0.72000000E 05		PSI 3= -0.64511999E 05		PSI 6= -0.38699996E 06	
PSI 3= C.10439999E 05		PSI 4= -C.17399999E 05		PSI 4= C.18719999E 05		PSI 7= C.41399997E 05	
PSI 4= -C.45449999E 03		PSI 5= 0.11999999E 04		PSI 5= -C.14399999E 04		PSI 8= -C.14399999E 04	

TABLE B-23 Ψ^u (n_1, p, n_2, d) (continued)

$n_1 = 2$		$n_2 = 7$		$(5,7)$ (continued)	
$n_1 = 4$		$n_2 = 7$		$n_1 = 4$	
PSI	0= C.719999999E 03	PSI	0= 0.25920004E 05	PSI	0= C.37439998E C4
PSI	1=-0.38399999E 04	PSI	1=-0.59256025E 06	PSI	1=-0.47039996E 05
PSI	2= 0.71499997E 04	PSI	2= C.47432540E 07	PSI	2= C.20591999E 06
PSI	3=-C.57599998E 04	PSI	3=-C.17607900E 08	PSI	3=-C.4147198L 06
PSI	4= 0.16799998E 04	PSI	4= 0.3356457dE 08	PSI	4= 0.4132800E 06
<u><u>$n_1 = 3$</u></u>	<u><u>$n_2 = 7$</u></u>	PSI	5=-C.3436065dE 08	PSI	5=-C.19526398E 06
PSI	0=-C.17999999E 04	PSI	6= C.19323358E 08	PSI	6= C.36000000E 01
PSI	1= C.13679999E 05	PSI	3=-C.25C90971E 07	PSI	7=-C.192000C5E C4
PSI	2=-0.34799999E 05	PSI	4= C.29375998E 07	PSI	8= C.38887981E 06
PSI	3= C.374400C0E 05	PSI	5=-0.16415037E 07	PSI	9=-C.68399992E 05
PSI	4=-C.16199997E 05	PSI	6= C.42825593E 06	PSI	10= C.16799992E 04
PSI	5= C.16799995E 04	PSI	7=-C.47519996E 05	<u><u>$n_1 = 2$</u></u>	<u><u>$n_2 = 5$</u></u>
<u><u>$n_1 = 4$</u></u>	<u><u>$n_2 = 7$</u></u>	PSI	8= 0.16799995E 04	PSI	0= C.719999999E 03
PSI	0= C.37439999E 04	PSI	1=-C.47999998E C4	PSI	4=-C.20518800E 07
PSI	1=-0.38351999E 05	PSI	2= C.11799999E 07	PSI	5= C.13318794E 07
PSI	2= C.14032000E 06	PSI	3=-0.14399999E C5	PSI	6=-0.40039200E 06
PSI	3=-C.16664776E 06	PSI	4= C.644C00000E 04	PSI	7= C.49749976E 05
PSI	4= C.11769600E 06	PSI	5=-C.19199999E 04	PSI	8=-C.1920005E C4
PSI	5=-C.26639996E 05	PSI	2=-C.231984C1E 07	<u><u>$n_1 = 3$</u></u>	<u><u>$n_2 = 5$</u></u>
PSI	6= C.168CC000E 04	PSI	3= C.70924762E 07	PSI	0=-C.17999999E 04
<u><u>$n_1 = 5$</u></u>	<u><u>$n_2 = 7$</u></u>	PSI	4=-C.10771439E 08	PSI	1= C.1692C000E 05
PSI	0=-C.68399997E 04	PSI	5= 0.83554399E 07	PSI	2=-C.56399999E 05
PSI	1= C.90007999E 05	PSI	6=-C.33297592E 07	PSI	3= 0.87599999E 05
PSI	2=-C.39664764E 06	PSI	7= 0.65856012E 06	PSI	4=-C.66549996E 05
PSI	3= 0.75700793E 06	PSI	8=-C.57959992E 05	PSI	5= C.22220000E 05
PSI	4=-0.65920000E C6	PSI	9= C.16799999E 04	PSI	6=-C.19199999E 04
				PSI	5=-0.72500612E 07

TABLE B-23 Ψ^u ($n_1 p, n_2 d$) (continued)

(5,8) (continued)		(8,8) (continued)		(3,9) (continued)		(3,9) (continued)		
PSI	6= 0.31862397E 07	PSI	10= 0.91199908E 05	PSI	2=-0.83159997E 05	PSI	0= C.11375999E 05	
PSI	7=-0.68198395E 06	PSI	11=-C.19200005E 04	PSI	3= 0.16920000E 06	PSI	1=-C.264096C1E 06	
PSI	8= 0.63600023E 05		<u>N1= 9</u>	PSI	4=-C.18540001E 06	PSI	2= 0.22102968E 07	
PSI	9=-C.19199985E 04	PSI	0=-0.36503921E 05	PSI	5= C.10800005E 06	PSI	3=-C.89169750E 07	
<u>N1= 7</u>	<u>N2= 8</u>	PSI	1= 0.11530785E 07	PSI	6=-C.29160000E 05	PSI	4= C.19323355E 08	
PSI	0=-C.17639998E 05	PSI	2=-C.13222446E 06	PSI	7= C.215999951E 04	PSI	5=-0.234018C9E 08	
PSI	1= C.41628003E 06	PSI	3= C.735888663E 08		<u>N1= 4</u>	<u>N2= 9</u>	PSI	6= 0.15767954E 08
PSI	2=-0.34920005E 07	PSI	4=-0.22246486E 09	PSI	0= C.37439998E 04		PSI	7=-C.56735965E 07
PSI	3= C.13831614E 08	PSI	5= 0.38344719E 09	PSI	1=-0.55727797E 05		PSI	8= C.10234080E 07
PSI	4=-C.28633880E 08	PSI	6=-C.39315830E 09	PSI	2= C.29879999E 06		PSI	9=-0.820779937E 05
PSI	5= 0.32099560E 08	PSI	7= 0.236942257E 09	PSI	3=-0.77399990E 06		PSI	10= C.215999980E 04
PSI	6=-0.19501512E 08	PSI	8=-C.85963519E 08	PSI	4= C.10706369E 07		PSI	
PSI	7= C.63191985E 07	PSI	9= C.17792282E 08	PSI	5=-C.80078400E 06		PSI	
PSI	8=-C.104004C1E 07	PSI	10=-0.19855437E 07	PSI	6= C.301967799E 06		PSI	
PSI	9= 0.77399953E 05	PSI	11= C.10500000E 06	PSI	7=-C.466800015E 05		<u>N1= 7</u>	<u>N2= 9</u>
PSI	10=-C.19199994E 04	PSI	12=-C.19199994E 04	PSI	8= C.215999707E 04		PSI	0=-C.17640000E 05
<u>N1= 8</u>	<u>N2= 9</u>	<u>N1= 2</u>	<u>N2= 9</u>		<u>N1= 5</u>	<u>N2= 9</u>	PSI	1= 0.48015996E 06
PSI	0= C.25920000E 05	PSI	0= C.71999999E 03	PSI	0=-0.68399997E 04		PSI	2=-0.490787795E 07
PSI	1=-C.71424022E 06	PSI	1=-0.57599998E 04	PSI	1= 0.12945599E 06		PSI	3= C.23474390E 08
PSI	2= C.70728689E 07	PSI	2= C.18C00000E 05	PSI	2=-C.87926397E 06		PSI	4=-0.63609228E 08
PSI	3=-0.33543763E 08	PSI	3=-0.28799998E 05	PSI	3= 0.2866847795E 07		PSI	5= 0.95980512E 08
PSI	4= 0.84833203E 08	PSI	4= C.25200007E 05	PSI	4=-0.499464C2E 07		PSI	6=-C.83253755E 08
PSI	5=-0.11977469E 09	PSI	5=-C.11519996E 05	PSI	5= C.47793590E 07		PSI	7= C.40924583E 08
PSI	6= 0.95980524E 08	PSI	6= 0.21599999E 04	PSI	6=-0.24413768E 07		PSI	8=-0.11063880E 08
PSI	7=-0.43708520E 06		<u>N1= 3</u>	PSI	7= 0.60710412E 06		PSI	9= C.15508777E 07
PSI	8= C.11073598E 08	PSI	0=-0.17999999E 04	PSI	8=-C.64440031E 05		PSI	10=-C.99720094E 05
PSI	9=-C.14745595E 07	PSI	1= 0.20159999E 05	PSI	9= C.215999980E 04		PSI	11= 0.21600009E 04

TABLE B-23 $\Psi^a(n_1 p, n_2 q)$
(continued)

<u>$n_1 = 8$</u>	<u>$n_2 = 9$</u>	<u>$n_1 = 3$</u>		<u>$n_2 = 5$</u>	<u>$n_1 = 3$</u>		<u>$n_2 = 5$</u>	<u>$n_1 = 3$</u>		<u>$n_2 = 5$</u>	<u>$n_1 = 3$</u>	
PSI 0= C.25920000E 05		PSI 0=	0.71999999E 03		PSI 0=	0.23447999E 06		PSI 0=	0.23447999E 06		PSI 0=	0.23447999E 06
PSI 1=-0.43592000E 06		PSI 1=-0.54000000E 04		PSI 1=-0.26567966E 06								
PSI 2= 0.98770639E 07		PSI 2= C.11231999E 05		PSI 2= C.12876000E 06								
PSI 3=-C.57271784E 08		PSI 3=-C.68399997E 04		PSI 3=-C.17639995E 05								
PSI 4= 0.18256140E 09		PSI 4= C.71999999E 03		PSI 4= C.12000000E 04								
PSI 5=-0.33699279E 09		PSI 5= C.71999999E 04		PSI 5= C.27719998E 05								
PSI 6= C.36763635E 09		PSI 6= C.22463969E 05		PSI 6= C.0.22463969E 06								
PSI 7=-0.23727106E 09		PSI 7=-C.27459999E 03										
PSI 8= 0.69552896E 08		PSI 8= C.11375999E 03		PSI 8= C.16031656E 07								
PSI 9=-0.19178636E 08		PSI 9=-C.13679999E 05		PSI 9=-C.70667995E 06								
PSI 10= C.21675193E 07		PSI 10= C.13679999E 05		PSI 10= C.17640000E 03								
PSI 11=-0.11736012E 06		PSI 11=-C.54526996E 03										
PSI 12= 0.21599970E 04		PSI 12= C.11375999E 05		PSI 12= C.56159997E 05								
<u>$n_1 = 9$</u>	<u>$n_2 = 9$</u>	<u>$n_1 = 3$</u>	<u>$n_2 = 7$</u>	<u>$n_1 = 3$</u>	<u>$n_2 = 5$</u>							
PSI 0=-C.36503921E 05		PSI 0= C.10127967E 05		PSI 0= C.71999999E 05								
PSI 1= 0.13476090E 07		PSI 1=-C.66815998E 03		PSI 1=-C.10583999E 06								
PSI 2=-C.18370783E 06		PSI 2= C.37440000E 05		PSI 2= C.56159997E 05								
PSI 3= C.12413094E 09		PSI 3=-C.68399998E 05		PSI 3=-C.17639998E 05								
PSI 4=-0.46694323E 09		PSI 4= C.17337235E 09										
PSI 5= 0.10347535E 10		PSI 5= C.30584303E 08		PSI 5= C.45023952E 06								
PSI 6=-C.13863236E 10		PSI 6=-C.11399037E 10		PSI 6=-C.16920000E 05								
PSI 7= C.11399037E 10		PSI 7= C.56879997E 05		PSI 7= C.60191917E 06								
PSI 8=-0.57269811E 09		PSI 8=-C.17639998E 05										
PSI 9= C.17337235E 09		PSI 9= C.30584303E 08		PSI 9= C.45023952E 06								
PSI 10= C.30584303E 08		PSI 10= C.13500000E 06		PSI 10= C.72864003E 06								
PSI 11= C.29393280E 07		PSI 11= C.21594960E 04										

TABLE 2-24 Ψ^j (n_1, d, n_2, p) (continued)

(4,8) (continued)		(3,9) (continued)		(continued)	
<u>$n_1 = 5$</u>	<u>$n_2 = 8$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 9$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 9$</u>
PSI 0=-C.227526004E 06		PSI 3=-0.239399999E 06		PSI 0=-C.143799994E 04	
PSI 7= 0.25920000E 05		PSI 4= C.39815997E 06		PSI 1= 0.56519999E 05	
<u>$n_1 = 5$</u>	<u>$n_2 = 8$</u>	PSI 5=-C.37064000E 06		PSI 2=-C.75535193E 06	
PSI 0= C.120000000E 04		PSI 6= C.16143994E 06		PSI 3= C.47131142E 07	
PSI 1=-C.328799992E 05		PSI 7=-0.36503968E 05		PSI 4=-0.15604702E 08	
PSI 2= 0.29879997E 06		<u>$n_1 = 6$</u>	<u>$n_2 = 9$</u>	PSI 5= 0.29046308E 04	
PSI 3=-0.12280881E 07		PSI 0=-C.959999997E 05		PSI 6=-C.30813827E 06	
PSI 4= C.25592569E 07		PSI 1= 0.23400000E 05		PSI 7= 0.18135075E 08	
PSI 5=-0.27828000E 07		PSI 2=-C.19506798E 06		PSI 8=-C.55036770E 07	
PSI 6= 0.15077822E 07		PSI 3= C.76626355E 06		PSI 9= C.76442450E 06	
PSI 7=-C.34920000E 06		PSI 4=-0.16203599E 07		PSI 10=-C.36503953E 05	
PSI 8= 0.25920016E 05		PSI 5= 0.19076359E 07		<u>$n_1 = 7$</u>	<u>$n_2 = 9$</u>
<u>$n_1 = 6$</u>	<u>$n_2 = 8$</u>	PSI 6=-C.12222001E 07		PSI 0= C.16799992E 04	
PSI 0=-0.14399999E 04		PSI 7= C.37576763E 06		PSI 1= -C.78839994E C5	
PSI 1= C.489599998E 05		PSI 8=-0.36503968E 05		PSI 2= 0.12642156E 07	
PSI 2=-0.55583993E 06				PSI 3=-C.96018460E 07	
PSI 3= 0.28684799E 07				PSI 4= C.36803676E C6	
PSI 4=-C.75669940E 07		PSI 0= C.11999999E 04		PSI 5=-0.89052904E 06	
PSI 5= 0.10638720E 08		PSI 1=-C.38039999E 05		PSI 6= 0.11876643E 09	
PSI 6=-0.78817342E 07		PSI 2= C.40895997E 06		PSI 7=-C.91454288E 08	
PSI 7= 0.288862287E 07		PSI 3=-C.20316156E 07		PSI 8= C.39337455E 08	
PSI 8=-0.47087981E 06		PSI 4= 0.54594237E 07		PSI 9=-0.89333980E 07	
PSI 9= 0.25920004E 05		PSI 5=-0.61194395E 07		PSI 10= C.95875049E 06	
<u>$n_1 = 3$</u>	<u>$n_2 = 9$</u>	PSI 6= C.67391995E 07		PSI 11=-C.36503984E 05	
PSI 0= 0.71999999E 03		PSI 7=-C.29332792E 07			
PSI 1=-0.12599999E 05		PSI 8= 0.57009537E 06			
PSI 2= C.78623996E 05		PSI 9=-0.36504000E 05			

TABLE B-25 Ψ^u ($n_1 d, n_2 f$)

<u>$n_1 = 3$</u>	<u>$n_2 = 4$</u>	<u>$n_1 = 3$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 7$</u>	<u>$n_2 = 6$</u>
PSI 0= 0.40319999E 05		PSI 0= 0.40319999E 05		PSI 0= C.36288003E 06	
<u>$n_1 = 4$</u>	<u>$n_2 = 5$</u>	<u>$n_1 = 4$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 7$</u>	<u>$n_2 = 6$</u>
PSI 0=-C.80639999E 05		PSI 1=-C.10079999E 06		PSI 1=-C.30499196E 07	
PSI 1= 0.40319999E 05		PSI 2= C.60479998E 03		PSI 2= 0.81679997E 07	
<u>$n_1 = 5$</u>	<u>$n_2 = 4$</u>	<u>$n_1 = 4$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 7$</u>	<u>$n_2 = 6$</u>
PSI 0= C.14399999E 06		PSI 0=-C.80639999E 05		PSI 0=-C.888031998E 06	
PSI 1=-0.16127999E 06		PSI 1= C.30239999E 06		PSI 1= C.60479998E 05	
PSI 2= C.40319999E 02		PSI 2=-0.29567999E 06		PSI 2=-0.49056000E 06	
<u>$n_1 = 3$</u>	<u>$n_2 = 5$</u>	<u>$n_1 = 4$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 5$</u>	<u>$n_2 = 6$</u>
PSI 0= 0.40319999E 05		PSI 0= 0.40319999E 05		PSI 0= 0.40319999E 05	
PSI 1=-0.50399999E 05		PSI 1=-0.50399999E 05		PSI 1=-0.50399999E 05	
<u>$n_1 = 4$</u>	<u>$n_2 = 5$</u>	<u>$n_1 = 5$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 6$</u>
PSI 0= 0.80639999E 05		PSI 0= 0.14399999E 06		PSI 0= 0.14399999E 06	
PSI 1= C.17135999E 06		PSI 1=-0.74591998E 06		PSI 1=-0.74591998E 06	
PSI 2=-C.50399999E 05		PSI 2= C.10434399E 07		PSI 2= C.10434399E 07	
<u>$n_1 = 5$</u>	<u>$n_2 = 5$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 6$</u>
PSI 0= 0.14399999E 06		PSI 0= 0.60479998E 05		PSI 0= 0.60479998E 05	
PSI 1=-0.45359999E 06		PSI 1=-0.45359999E 06		PSI 1=-0.45359999E 06	
PSI 2= C.30239999E 06		PSI 2= C.30239999E 06		PSI 2= C.30239999E 06	
PSI 3=-C.50400000E 05		PSI 3=-C.50400000E 05		PSI 3=-C.50400000E 05	
<u>$n_1 = 6$</u>	<u>$n_2 = 5$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 6$</u>	<u>$n_1 = 6$</u>	<u>$n_2 = 6$</u>
PSI 0=-0.23615998E 06		PSI 0=-C.23615999E 06		PSI 0=-C.23615999E 06	
PSI 1= C.10123200E 07		PSI 1= C.15426399E 07		PSI 1= C.15426399E 07	
PSI 2=-C.11188799E 07		PSI 2=-0.324886399E 07		PSI 2=-0.324886399E 07	
PSI 3= 0.43344000E 06		PSI 3= C.24134400E 07		PSI 3= C.24134400E 07	
PSI 4=-C.20399999E 05		PSI 4=-0.68244001E 06		PSI 4=-0.68244001E 06	
		PSI 5= 0.60479998E 05		PSI 5= 0.60479998E 05	

TABLE B-26 $\Psi^u_{(n_1, f, n_2)}$

<u><u>$n_1 = 4$</u></u>		<u><u>$n_2 = 6$</u></u>		<u><u>$n_1 = 5$</u></u>		<u><u>$n_2 = 6$</u></u>		<u><u>$n_1 = 5$</u></u>		<u><u>$n_2 = 7$</u></u>	
PSI	0 = C. 40319999E 0	PSI	0 = -C. 50399999E 0	PSI	0 = -C. 50399999E 0	PSI	0 = -C. 50399999E 0	PSI	0 = -C. 50399999E 0	PSI	0 = -C. 50399999E 0
PSI	1 = -C. 24191999E 0	PSI	1 = C. 69251999E 0	PSI	1 = C. 69251999E 0	PSI	1 = C. 69251999E 0	PSI	1 = C. 69251999E 0	PSI	1 = C. 69251999E 0
PSI	2 = C. 43200000E 0	PSI	2 = -C. 35263998E 0	PSI	2 = -C. 35263998E 0	PSI	2 = -C. 46686399E 0	PSI	2 = -C. 46686399E 0	PSI	2 = -C. 46686399E 0
PSI	3 = -C. 23615999E 0	PSI	3 = C. 72431999E 0	PSI	3 = C. 72431999E 0	PSI	3 = C. 13766400E 0	PSI	3 = C. 13766400E 0	PSI	3 = C. 13766400E 0
<u><u>$n_1 = 4$</u></u>		<u><u>$n_2 = 7$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 6$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 7$</u></u>	
PSI	0 = C. 40319999E 0	PSI	5 = C. 35928000E 0	PSI	5 = C. 35928000E 0	PSI	5 = C. 16113599E 0	PSI	5 = C. 16113599E 0	PSI	5 = C. 16113599E 0
PSI	1 = -C. 32255999E 0	PSI	6 = -C. 52791994E 0	PSI	6 = -C. 52791994E 0	PSI	6 = -C. 60177560E 0	PSI	6 = -C. 60177560E 0	PSI	6 = -C. 60177560E 0
<u><u>$n_1 = 5$</u></u>		<u><u>$n_2 = 6$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 6$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 7$</u></u>	
PSI	2 = 0. 86399999E 0	PSI	0 = C. 60474999E 0	PSI	0 = C. 60474999E 0	PSI	7 = C. 74304000E 0	PSI	7 = C. 74304000E 0	PSI	7 = C. 74304000E 0
PSI	3 = -0. 94464000E 0	PSI	1 = -C. 10751994E 0	PSI	1 = -C. 10751994E 0	PSI	0 = C. 60474999E 0	PSI	0 = C. 60474999E 0	PSI	0 = C. 60474999E 0
<u><u>$n_1 = 5$</u></u>		<u><u>$n_2 = 7$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 7$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 8$</u></u>	
PSI	4 = C. 36287996E 0	PSI	2 = C. 66403195E 0	PSI	3 = -C. 16777600E 0	PSI	1 = -C. 127008C0E 0	PSI	1 = -C. 127008C0E 0	PSI	1 = -C. 127008C0E 0
PSI	5 = -0. 50399999E 0	PSI	4 = C. 26553598E 0	PSI	4 = C. 26553598E 0	PSI	2 = C. 95471992E 0	PSI	2 = C. 95471992E 0	PSI	2 = C. 95471992E 0
PSI	6 = C. 56448000E 0	PSI	5 = C. 1606E480E 0	PSI	5 = C. 1606E480E 0	PSI	3 = -0. 34509439E 0	PSI	3 = -0. 34509439E 0	PSI	3 = -0. 34509439E 0
PSI	7 = -C. 20764799E 0	PSI	6 = C. 53712004E 0	PSI	6 = C. 53712004E 0	PSI	4 = C. 65294404E 0	PSI	4 = C. 65294404E 0	PSI	4 = C. 65294404E 0
PSI	8 = 0. 51452798E 0	PSI	7 = -C. 52492006E 0	PSI	7 = -C. 52492006E 0	PSI	5 = -0. 67385276E 0	PSI	5 = -0. 67385276E 0	PSI	5 = -0. 67385276E 0
PSI	9 = -C. 19972799E 0	PSI	8 = C. 36287996E 0	PSI	8 = C. 36287996E 0	PSI	6 = C. 361756E5E 0	PSI	6 = C. 361756E5E 0	PSI	6 = C. 361756E5E 0
<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 8$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 8$</u></u>		<u><u>$n_1 = 6$</u></u>		<u><u>$n_2 = 9$</u></u>	
PSI	0 = C. 40319999E 0	PSI	1 = -C. 40319999E 0	PSI	1 = -C. 40319999E 0	PSI	2 = C. 21599999E 0	PSI	2 = C. 21599999E 0	PSI	2 = C. 21599999E 0
PSI	1 = -C. 40319999E 0	PSI	2 = C. 14399999E 0	PSI	3 = -C. 47231998E 0	PSI	3 = -C. 47231998E 0	PSI	3 = -C. 47231998E 0	PSI	3 = -C. 47231998E 0
PSI	2 = C. 14399999E 0	PSI	3 = -C. 23616000E 0	PSI	4 = C. 54431999E 0	PSI	5 = -C. 31795195E 0	PSI	5 = -C. 31795195E 0	PSI	5 = -C. 31795195E 0
PSI	3 = -C. 23616000E 0	PSI	4 = 0. 18143997E 0	PSI	6 = C. 74304025E 0	PSI	7 = C. 74304025E 0	PSI	8 = C. 74304025E 0	PSI	9 = C. 74304025E 0

TABLE B-27
TRANSITION INTEGRAL σ^2

Atom	Transition Integral σ^2		
	Hydrogenic	Coulomb Approx.	Hartree-Fock
Be I	2.27	2.03	1.86
B II	0.977	1.010	
C III	0.544	0.573	
N IV	0.348	0.368	
P XII	0.0522	0.0540	

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APPENDIX C
D. Layzer

NEW GENERALIZATION OF THE SCREENING THEORY
AND THE HARTREE-FOCK THEORY

C.1. Introduction

The distinguishing feature of the Z -dependent theory of atomic spectra (Layzer,^(C-1)) henceforth referred to as A) is the fact that it allows for certain effects of configuration mixing in the first approximation. This ensures that the predicted term energies have the correct linear dependence on Z . Experiment shows that the structure of term spectra, in both simple and complex systems, depends strongly on the linear Z -dependence of the energies. A knowledge of the energy coefficients W_2 and W_1 in the expansions

$$W = W_2 Z^2 + W_1 Z + W_0 + O(Z^{-1}) \quad (C-1)$$

enables one to describe quantitatively the most conspicuous features of term spectra in isoelectronic sequences (see especially Figures 1 and 2 in reference C-1).

In order to calculate the coefficients W_1 (W_2 is given by the well-known hydrogenic formula) one needs to know nothing about the radial dependence of the atomic charge distribution beyond what is provided by the theory of the hydrogen atom. That is, all the necessary calculations utilize hydrogenic wavefunctions. One can, of course, use less simple wavefunctions in these calculations, as was done in the first calculations of this type (Layzer^(C-2)), but such refinements only improve the accuracy of higher terms in the expansion.

For some purposes, however, one does require a reasonably accurate knowledge of the radial charge distribution and hence of the radial wavefunctions. One needs this information, for example, in order to calculate electric-dipole transition probabilities.

The various procedures in common use for calculating accurate radial wavefunctions are all based on the variation principle. They differ through the restrictions they impose on the form of the variational functions. Hartree-Fock wavefunctions (i.e., exact solutions of the Hartree-Fock integro-differential equations) fall at one end of the gamut of variational wavefunctions, screened hydrogenic wavefunctions at the other. The latter involve only a single adjustable parameter, while the former are restricted beforehand only by the usual conditions of integrability and smoothness. Other types of variational wavefunctions seek to achieve some of the accuracy of Hartree-Fock wavefunctions without sacrificing all the simplicity of screened hydrogenic wavefunctions. Which type of variational wavefunction one chooses to employ will be governed by the purpose in view. The Hartree-Fock description is certainly the most accurate; from a qualitative standpoint, however, the screening description offers unrivalled advantages of simplicity and flexibility.

Any meaningful comparison between different variational wavefunctions presupposes a common approximation scheme. Thus we may compare wavefunctions calculated with neglect of configuration mixing, or with certain specified kinds

of configuration mixing taken into account. (In practice, the calculations that allow most fully for configuration mixing are those based on the simplest wavefunctions, so that strict comparisons are difficult.)

According to the Z-dependent theory, the most important kind of configuration mixing is that between configurations belonging to the same complex (i.e., the same set of principal quantum numbers and the same parity). On the other hand, the theory of radial wavefunctions has usually been developed within the framework of the central-field approximation, though attempts have occasionally been made to allow for effects of configuration mixing. A notable example is the work of Hartree, Hartree, and Swirles (C-3), which dealt with the mixing of configurations $1s^2 2s^2 2p^n$ with configurations $1s^2 2p^{n+2}$. However, such attempts have lacked an adequate theoretical framework, comparable in simplicity and generality with that provided by the central-field approximation. The present paper seeks to supply such a framework.

C.2. The Theoretical Framework

Let Ψ denote an antisymmetric N-electron wavefunction pertaining to a definite state in a definite electronic configuration. The quantity

$$W = \langle \Psi H \Psi \rangle , \quad (C-2)$$

where H is the N-electron Hamiltonian and the brackets $\langle \rangle$ indicate an integration over all $3N$ coordinates and a summation over all the spin variables, is the variational ener-

gy. It is a functional of the radial wavefunctions. If these are specified beforehand, except for the values of certain parameters, then W reduces to a function of these parameters. W exceeds the true energy of the state under consideration provided that Ψ is normalized and is orthogonal to the true eigenfunctions of all states lower than the one under consideration. The condition $\delta W = 0$ leads to a set of simultaneous integro-differential equations for the radial wavefunctions, or to a set of simultaneous algebraic equations for the adjustable parameters.

One can easily generalize the theory just sketched so as to include the effects of mixing among a finite number of configurations. Let $\Psi_1, \Psi_2, \dots, \Psi_r$ denote variational wavefunctions for states with fixed values of the quantum numbers SLp in different configurations. Suppose, for the sake of definiteness, that Ψ_1 corresponds to the deepest of the states under consideration. Then the corresponding variational energy W^1 is the lowest eigenvalue of the matrix $\|\langle \Psi_i | H | \Psi_j \rangle\|$. As before, the condition $\delta W^1 = 0$ yields a set of simultaneous equations for the unknown functions or parameters. (Note that all the radial wavefunctions or parameters that figure in the complete set Ψ_1, \dots, Ψ_r may occur in a single equation.)

An accurate solution of the secular equation for W^1 would lead to a set of variational equations of prohibitive complexity. The procedure usually adopted consists in retaining only first- and second-order contributions to W^1 , in the sense of ordinary perturbation theory. Thus W^1 is

given by

$$W^1 = \langle \Psi_1 | H | \Psi_1 \rangle + \sum_{i \neq 1} \frac{|\langle \Psi_1 | H | \Psi_i \rangle|^2}{E_1 - E_i}, \quad (C-3)$$

where E_i denotes the mean energy of the i th configuration. Even with this simplification, the variational equations with configuration mixing taken into account present considerable more difficulty than the usual equations. And frequently the effects of mixing are so large that second-order perturbation theory does not describe them adequately.

Another important difficulty inherent in the usual methods of dealing with configuration mixing concerns the choice of interacting configurations. It is of course true that the more interactions one takes into account, the more accurate will be the theoretical description. It has been amply demonstrated, however, that in order to obtain predictions of term spacing in neutral and slightly ionized systems that are accurate to within a few percent, one needs to allow for a very large number of interactions. Hence a calculation that allows for mixing between a small number of configurations would be significant only if the choice of the configurations considered could be justified on grounds other than mathematical convenience.

The problem of configuration mixing takes on a different complexion if we adopt the Z -dependent approach. Consider the expansion

$$\Psi = \sum_i a_i \Psi_i , \quad (C-4)$$

where the Ψ_i refer to distinct configurations and the sum runs over all configurations connected with configuration 1 (say) by nonvanishing energy matrix elements, (we assume that the state corresponding to Ψ has been nominally assigned to configuration 1).

The numerical values of the coefficients a_i depend on the choice of radial wavefunctions. For example, if the radial wavefunctions in Ψ_1 are solutions of the Hartree-Fock equations, then the coefficients a_i pertaining to configurations with the same set of azimuthal quantum numbers as configuration 1 will all be very small, because the variation principle ensures that most of the effects of mixing between configurations characterized by the same set of azimuthal quantum numbers have already been incorporated in the wavefunctions. Now, every coefficient a_i is either $O(1)$ or $O(z^{-1})$. The coefficients of the first type are associated with configurations that have the same set of principal quantum numbers as configuration 1; those of the second type with configurations that have a different set of principal quantum numbers.

The coefficients of the first type can be written in the form

$$a_i = a_i^0 + O(z^{-1}) , \quad (C-5)$$

where a_i^0 is independent of z . It was shown in A that the

constants a_i^0 do not depend on the form of the radial wavefunctions. The coefficients and parts of coefficients that do depend on the form of the radial wavefunctions are $O(z^{-1})$.

We may conveniently split off the terms on the right side of (C-4) that have constant coefficients:

$$\psi = \sum_i a_i^0 \psi_i + \sum_i a'_i \psi_i, \quad (C-6)$$

where

$$a'_i = a_i - a_i^0 = O(z^{-1}). \quad (C-7)$$

The nonvanishing coefficients a_i^0 are finite in number. They can be calculated with arbitrary precision, being essentially by-products of the calculation that yields the energy coefficients W_1 (see A).

We propose to replace the usual approximation, which consists in neglecting configuration interaction entirely, by an approximation that represents the wavefunction for a given state by the finite sum

$$\psi = \sum_i a_i^0 \psi_i, \quad (C-8)$$

where the coefficients may be regarded as known numbers. (For spectroscopic terms belonging to complexes of the type $(1^2 2^q)$ and $(1^2 2^q)^0$ they are given in Table C-1.

The approximation just described becomes increasingly accurate as Z increases along an isoelectronic sequence.

TABLE C-1
CONFIGURATION MIXING COEFFICIENTS

Complex	Configuration	Configuration	Term	$\langle ar r \rangle$	$\langle ar t \rangle$	$\langle ar E \rangle$
$(1^2_2)^2$	20	02	r			
$(1^2_2)^3$	21	03	t			
$(1^2_2)^4$	22	04	r	.974320628	.225165081	.231099573
			t	.986327360	.164797870	.167082327
			r	.994467221	-.105047356	-.105631793
			t	.979686046	-.200537408	-.204695585
$(1^2_2)^5$	23	05	r	.991349355	.131249594	.132394895
$(1^2_2)^6$	24	06	t	.989539014	.144265516	.145790630

Even for moderately ionized and un-ionized systems, however, it should prove superior to the central-field approximation, since experiment has shown that the linear Z-dependence of the term energies usually dominates the structure of the term spectrum.

C.3. The Generalized Screening Parameters

Notation. The letters r, t, t' will denote configurations; the symbol Γ will distinguish different states in the same configuration; a will denote an orbital nl ; and \underline{a} will denote a complex. Thus the label $a(r)\Gamma$ distinguishes the state Γ nominally assigned to the configuration r of the complex \underline{a} . In the present notation, equation (C-4) takes the form

$$\Psi(ar\Gamma) = \sum_t \langle ar\Gamma | t\Gamma \rangle \Psi(t\Gamma) . \quad (C-9)$$

The Hamiltonian H for a many-electron system is given, in the nonrelativistic approximation, by

$$H = H_0 + V , \quad (C-10)$$

where

$$H_0 = \sum_i \left(-p_i^2/2m - ze^2/r_i \right) , \quad (C-11)$$

$$V = \sum_{i < j} e^2/r_{ij} . \quad (C-12)$$

The variational energy in the present approximation is defined as

$$W = \langle ar\Gamma' | H | ar\Gamma' \rangle . \quad (C-13)$$

We now evaluate W using screened hydrogenic wavefunctions for the undetermined radial wavefunctions that figure in this formula.

For the one-electron part of W we obtain

$$\begin{aligned} \langle ar\Gamma | H_0 | ar\Gamma \rangle &= \sum_{t,t'} \langle ar\Gamma | t\Gamma \rangle \langle t\Gamma' | H_0 | t'\Gamma' \rangle \langle t'\Gamma' | ar\Gamma \rangle \\ &= \sum_t |\langle ar\Gamma | t\Gamma \rangle|^2 \langle t\Gamma | H_0 | t\Gamma \rangle \\ &= \sum_t |\langle ar\Gamma | t\Gamma \rangle|^2 \left(\sum_{\alpha} q_{\alpha t} (-z^2 + s_{\alpha t}^2) / 2n_{\alpha}^2 \right) , \end{aligned} \quad (C-14)$$

where $q_{\alpha t}$ denotes the number of orbitals of type α in the configuration t , and $s_{\alpha t}$ denotes the screening parameter that corresponds to the orbital α in configuration t . A more complete notation for this screening parameter is $s_z(\alpha t | r\Gamma)$. The suffix Z indicates that the screening parameter depends in general on Z ; s_z differs from s_{∞} by terms $O(z^{-1})$. The labels $r\Gamma'$ indicate that the value of the screening parameter depends on the state under consideration.

For the two-electron contribution to W we have

$$\langle ar\Gamma|v|ar\Gamma\rangle = \sum_{t,t'} \langle ar\Gamma|t\Gamma\rangle \langle t\Gamma|v|t'\Gamma\rangle \langle t'\Gamma|ar\Gamma\rangle . \quad (C-15)$$

Hence

$$\begin{aligned} \langle ar\Gamma|H|ar\Gamma\rangle = \sum_t |\langle ar\Gamma|t\Gamma\rangle|^2 & \left[\sum_a q_{at} (-z^2 + s_{at}^2/2n_a^2) + \right. \\ & \left. + \sum_{t'} \frac{\langle t'\Gamma|ar\Gamma\rangle}{\langle t\Gamma|ar\Gamma\rangle} \langle t\Gamma|v|t'\Gamma\rangle \right] . \end{aligned} \quad (C-16)$$

The variational equations are

$$\frac{\partial W}{\partial s_{at}} = \frac{q_{at} s_{at}}{n_a^2} - \frac{\partial}{\partial z_{at}} (\langle t\Gamma|v|t\Gamma\rangle + 2 \sum_{t' \neq t} c_{tt',r\Gamma} \langle t\Gamma|v|t'\Gamma\rangle) = 0 . \quad (C-17)$$

where

$$z_{at} = z - s_{at} , \quad c_{tt',r\Gamma} = \langle t'\Gamma|ar\Gamma\rangle / \langle t\Gamma|ar\Gamma\rangle . \quad (C-18)$$

The diagonal matrix element $\langle t\Gamma|v|t\Gamma\rangle$ may be written in the form

$$\langle t\Gamma|v|t\Gamma\rangle = v_t + v_{t\Gamma} , \quad (C-19)$$

where the contribution v_t represents the average value of $\langle t\Gamma|v|t\Gamma\rangle$. Explicitly,

$$v_t = \frac{\sum_{aSL} \langle taSL|v|taSL\rangle (2s+1)(2L+1)}{\sum_{aSL} (2s+1)(2L+1)} . \quad (C-20)$$

The term-dependent contribution $v_{t\Gamma}$ vanishes when the configuration t consists of complete groups only, or of complete groups plus or minus a single electron. The contribution to $v_{t\Gamma}$ from interactions between electrons in a group l^n satisfies the symmetry condition

$$v(l^n\Gamma) = v(l^{4l+2-n}\Gamma) . \quad (C-21)$$

In a first approximation one may wish to neglect the term-dependence of the screening parameters. We accordingly define

$$s(at) = \frac{n^2}{q_a} \frac{\partial v_t}{\partial z_{at}} . \quad (C-22)$$

If the configuration t contains no more than one incomplete group, v_t can be put in the form

$$v_t = \sum_{\alpha\beta} q_{\alpha\beta} (\alpha\beta) , \quad (C-23)$$

where

$$q_{\alpha\beta} = \begin{cases} \binom{q_\alpha}{2} & (\alpha = \beta) \\ \frac{q_\alpha q_\beta}{2} & (\alpha \neq \beta) \end{cases} \quad (C-24)$$

The two-electron interaction $(\alpha\beta)$ is defined in A; in a first approximation $(\alpha\beta) \approx F^0(\alpha\beta)$. The coefficient $q_{\alpha\beta t}$ denotes the number of ways in which two electrons labelled by the indicated quantum numbers can be selected from the configuration t .

With the help of these definitions we can write $s(at)$ in the form

$$s(at) = \sum_{\beta} (q_{\beta} - \delta_{\alpha\beta}) s(\alpha|\beta) , \quad (C-25)$$

where

$$s(\alpha|\beta) = (1 - \frac{1}{2}\delta_{\alpha\beta}) n_{\alpha}^2 \frac{\partial}{\partial z_{\alpha}} (\alpha\beta) . \quad (C-26)$$

The two-electron screening parameter $s(\alpha|\beta)$ provides an unambiguous, quantitative measure of the screening of an α electron by a β electron.

The screening parameters $s_{\infty}(\alpha|\beta)$ are independent of the configuration t , and can therefore be evaluated once and for all.

The exact screening parameters are given by

$$s(at|r\Gamma) = s(at) + \frac{n_{\alpha}^2}{q_{\alpha}} \frac{\partial}{\partial z_{at}} (v_{t\Gamma} + 2 \sum_{t' \neq t} c_{tt',r\Gamma} v_{tt',\Gamma}) , \quad (C-27)$$

where

$$v_{tt',\Gamma} = \langle t\Gamma | v | t'\Gamma \rangle . \quad (C-28)$$

In this equation one is not in general justified in neglecting the contribution from configuration mixing. In some instances the second term in the brackets () may be considerably larger than the first term. This is always the case, for example, when the configuration t is composed of complete groups but contains one or more incomplete shells, e.g., $1s^2 2s^2$. Then $v_{t\Gamma} = 0$, but $v_{tt',\Gamma} \neq 0$.

The set of equations (C-27) for all orbitals α in the mixture (C-9) determines the corresponding screening parameters $s_Z(\alpha t | r\Gamma)$. In spite of their complicated appearance, these equations are comparatively easy to solve numerically. In practice one uses an iterative procedure, first evaluating the right sides for $Z = \infty$. This gives the screening constants $s_\infty(\alpha t | r\Gamma)$. In the next approximation one evaluates the right sides for finite values of Z , replacing the parameters s by the constants s_∞ , and so on.

One can take advantage of the dominant contribution of $s(\alpha t)$ to $s(\alpha t | r\Gamma)$ to shorten the iterative evaluation of Z -dependent screening parameters. One begins by solving the system of equations (C-22) for $s_Z(\alpha t)$. One then evaluates the term-dependent correction to $s_Z(\alpha t | r\Gamma)$ using $s_Z(\alpha t)$ in place of $s_Z(\alpha t | r\Gamma)$ in equation (C-27). With this method one needs to go through the iterative procedure only once for a given configuration.

C.4. Generalized Hartree-Fock Theory

The Hartree-Fock equations may be written in the form

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Z - Y_{nl}}{r} \right) p_{nl} = E_{nl} p_{nl} + \frac{X_{nl}}{r}. \quad (C-29)$$

The quantities Y_{nl} and X_{nl} are functionals of all the radial wavefunctions appropriate to the configuration being considered. The exchange term X_{nl} has its origin in the antisymmetry of many-electron wavefunctions.

If we take as our starting point the approximation (C-9)

instead of the central-field approximation, we arrive at an equation that is formally identical with (C-29). This equation differs, in fact, from the ordinary Hartree-Fock equation only through the exchange term X_{nl} , which contains additional contributions arising from configuration mixing. These contributions are of precisely the same type as the ordinary exchange contributions. Thus the increase in accuracy that results from allowing for the dominant effects of configuration mixing has not been bought at the price of added complexity.

There exists a very close analogy between the Hartree-Fock theory and the hydrogenic screening theory, which it is convenient to exploit because the screening theory is so much simpler than the Hartree-Fock theory. The generalized Hartree-Fock equations are analogous to the screening equations (C-27). Just as in the screening theory one is not justified in neglecting the mixing contributions of $v_{tt'\Gamma}$ beside the term-dependent contributions $v_{t\Gamma}$, so in the generalized Hartree-Fock theory one is not justified in neglecting the mixing contributions to X_{nl} .

Calculations based on the generalized Hartree-Fock theory are planned for the near future.

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APPENDIX D
D. Layzer

APPLICABILITY OF THE SCREENING THEORY TO HEAVY ATOMS

D.1. Introduction

In the following, the term "screening theory" will be used to designate the Z-dependent approximation scheme described by Layzer ^(D-1) and, in a generalized form that allows fully for relativistic effects, by Layzer and Bahcall ^(D-2). The term "Slater theory" will be used to designate the conventional theory of atomic spectra, whose basic approximations were introduced by Slater in his classic paper of 1929. ^(D-3) Slater's ^(D-4) recent two-volume monograph, "Quantum Theory of Atomic Structure", describes the modern form of the theory.

The screening theory was devised to account for certain systematic discrepancies between the Slater theory and experiment, pertaining to the centers of gravity of spectroscopic terms. These discrepancies are sometimes large enough to reverse the predicted order of term energies in a configuration.

Now, any reasonably general theory of atomic structure must incorporate some fairly drastic simplifying assumptions. The Slater theory rests on the assumption that the effects of configuration mixing can be neglected in a first approximation. The screening theory, on the other hand, rests on the assumption that the energy of an atomic system can be expressed as a rapidly convergent power series in $(Z - s)^{-1}$, where Z is the nuclear charge and s is a screening parameter. This assumption leads naturally to a theory that is in most respects simpler than the Slater theory, but which allows for certain effects of configuration mixing in the first approximation.

As yet, the screening theory has been applied only to light atoms -- specifically to atoms with ten or fewer electrons. In these applications it has proved very successful, accounting in a quantitative way for features of term spectra that the Slater theory describes only semi-quantitatively or qualitatively. The question now arises whether the screening theory will also provide a useful description of the spectra of heavy atoms. The answer hinges on how rapidly expansions of the term energies in inverse powers of $Z - s$ converge. The fact that $Z - s$ increases with N (the number of atomic electrons) argues for the applicability of the theory to heavy atoms. On the other hand, one would also expect the coefficients in the energy expansion to increase with N . Since it is far from obvious to what extent the second effect will offset the first, the question cannot be decided with confidence on general grounds; specific calculations are required.

The iron-group elements provide ideal subjects for such calculations. They are sufficiently heavy to afford a definitive test. At the same time, they are sufficiently light to enable relativistic contributions to the energy to be treated as perturbations. Finally, the spectra of many atoms and ions in the iron group have been well analysed experimentally.

In evaluating the merits of a theoretical description, one must compare it not only with the data it sets out to describe but also with other available theoretical descriptions. During the past few years, attempts have been made to patch up the Slater theory, as it applies to the spectra of elements in the iron group, by adding to the theoretical energy formulae

an empirical correction term of the form $\alpha L(L + 1)$. That a term of this type could account for a fairly large part of the discrepancy between the Slater theory and experiment, in spectra of the iron group, was first pointed out by Layzer^(D-5) and, independently, by Racah.^(D-6) The Slater theory, amended in this way, has since been used extensively by Trees, Rohrlich, and Racah and his pupils in semi-empirical analyses of term spectra in the iron group. Racah^(D-7) has suggested that a theoretical basis for the $L(L + 1)$ correction is afforded by the work of Bacher and Goudsmit.^(D-8)

In the following, we shall re-examine the theoretical basis of the $L(L + 1)$ correction. We shall also present the results of new calculations, based on the screening theory, for complexes with a partly filled M shell. We shall find that the modified Slater theory cannot account quantitatively for the effects of configuration mixing described by the screening theory. We shall also find that the latter are of the same order of magnitude as the observed discrepancies. This suggests that the screening theory will provide an adequate description of these spectra. Unfortunately, sufficient experimental data are not yet available to test the theoretical calculations presented here, the complexes here studied having been chosen for their comparative mathematical simplicity rather than for comparison with experiment. However, work now in progress should lead before long to a definitive experimental test of the screening theory as applied to atoms and ions in the iron group.

D.2. Theoretical Results for Complexes with a Partly-Filled M Shell*

We have considered the following complexes: $(1^2 2^8 3^2)$, $(1^2 2^8 3^2)^0$, $(1^2 2^8 16)$, $(1^2 2^8 16)^0$. The configurations belonging to these complexes are listed in Table D-1. These are the simplest complexes with partly-filled M shells, other than those consisting of closed shells plus or minus a single electron. Complexes containing from three to seven 3d electrons present a somewhat more difficult theoretical problem.

The evaluation of the energy coefficients W_1 and the unitary matrices that diagonalize the energy submatrices $V_{(n)pSL}$ proceeds along the lines laid down in the reference cited earlier (Layzer (D-1)). [W_1 is the coefficient of Z in an expansion of the nonrelativistic part of the energy in inverse powers of Z ; $V_{(n)pSL}$ is a finite matrix whose elements connect states labelled by the indicated quantum numbers. W_1 is an eigenvalue of $V_{(n)pSL}$, the radial integrals that figure in the matrix elements being evaluated with straight hydrogenic wavefunctions.]

The results of the calculation are present in Tables D-2 thru D-9. Tables D-2 thru D-5 give the coefficients W_1 as well as the values that would have been obtained for these coefficients if configuration interaction had been neglected (i.e., the values of W_1 according to the Slater theory). Tables D-6 thru D-9 give the unitary matrices that diagonalize the various energy submatrices $V_{(n)pSL}$.

* The work summarized in this subsection was supported in part by a grant from the National Science Foundation.

TABLE D-1
TERMS AND CONFIGURATIONS FOR COMPLEXES WITH A
PARTIALLY FILLED M SHELL

Complex	Configuration	Terms
$(1^2 2^8 3^2)$	$1s^2 2s 2p^6 3s^2$ $3s 3d$ $3p^2$ $3d^2$	1S $^1D, ^3D$ $^1S, ^3P, ^1D$ $^1S, ^3P, ^1D, ^3F, ^1G$
$(1^2 2^8 3^{16})$	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8$ $3s^2 3d^{10}$ $3s 3p^5 3d^{10}$ $3p^1 3d^{10}$	$^1S, ^3P, ^1D, ^3F, ^1G$ $^1S, ^3P, ^1D$ $^1D, ^3D$ 1S
$(1^2 2^8 3^2)^o$	$1s^2 2s^2 2p^6 3s 3p$ $3p 3d$	$^1P, ^3P$ $^1P, ^3P, ^1D, ^3D, ^1F, ^3F$
$(1^2 2^8 3^{16})^o$	$1s^2 2s^2 2p^6 3s^2 3p^5 3d^9$ $3s 3p^5 3d^{10}$	$^1P, ^3P, ^1D, ^3D, ^1F, ^3F$ $^1P, ^3P$

TABLE D-2

W_1' in $(1^2 2^8 3^2)$. W_1' is the term-dependent part of W_1 ; $W_1 = \bar{W}_1 + W_1'$. (W_1') _{c.f.} denotes the value of W_1' obtained when configuration mixing is neglected.

Configuration	Term	W_1'	(W_1') _{c.f.}	$W_1' - (W_1')$ _{c.f.}
$3s^2$	1S	-.00357	0	-.00357
$3s3d$	3D	-.00228	-.00228	-
	1D	.01581	.00684	.00897
$3p^2$	3P	-.00481	-.00432	-.00049
	1D	-.00560	.00432	-.00992
$3d^2$	1S	.01748	.01727	.00021
	3P	-.00564	-.00564	-
	1D	.00295	.00201	.00094
	3P	.00373	.00322	.00051
	1G	.00616	.00616	-
	1S	.02719	.02382	.00337

TABLE D-3
 w_1' in $(1^2 2^8 3^2)^o$ (See Table D-2)

Config.	Term	w_1'	(w_1') c.f.	$w_1' - (w_1')$ c.f.
3s 3p	$^1P^o$.01801	.02116	-.00315
	$^3P^o$	-.00753	-.00705	-.00048
3p 3d	$^1P^o$.02215	.01900	.00315
	$^3P^o$.00255	.00207	.00048
	$^1D^o$	-.00869	-.00869	-
	$^3D^o$.00086	.00086	-
	$^1F^o$.01934	.01934	-
	$^3F^o$	-.00859	-.00859	-

TABLE D-4

w_1' in $(1^2 2^8 3^{16})$. (See Table D-2)

Configuration Term		w_1'	(w_1') cf	$w_1' - (w_1')$ cf
$3p^6 3d^{10}$	1s	.00262	0.	+.002620
$3s 3p^6 3d^9$	3D	-.00228	-.00228	----
	1D	.01926	.00684	+.012424
$3s^2 3p^4 3d^{10}$	3P	-.00406	-.00432	+.000258
	1D	-.00763	.00432	-.011951
	1S	.01625	.01727	-.001024
$3s^2 3p^6 3d^8$	3F	-.00564	-.00564	----
	1D	.00154	.00201	-.000472
	3P	.00296	.00322	-.000258
	1G	.00616	.00616	----
	1S	.02226	.02382	-.001595

TABLE D-5
 w_1' in $(1^2 2^8 3^{16})$. (See Table D-2)

Configuration Term	w_1'	$(w_1')_{cf}$	$w_1' - (w_1')_{cf}$
$3s\ 3p^5\ 3d^{10}$			
1_p^0	.02281	.02116	.001649
3_p^0	-.00678	-.00705	.000274
$3s^1\ 3p^5\ 3d^9$			
1_p^0	.01735	.01900	-.001649
3_p^0	.00180	.00207	-.000274
1_d^0	-.00869	-.00869	----
3_d^0	.00086	.00086	----
1_f^0	.01934	.01934	----
3_f^0	-.00859	-.00859	----

TABLE D-6
THE UNITARY MATRICES $|\langle \mathbf{r}\Gamma | \mathbf{t}\Gamma \rangle|$ $(1^2 2^8 3^2)$

1s

New	Old	$3s^2$	$3p^2$	$3d^2$
	$3s^2$.99031	.13789	-.01670
	$3p^2$	-.13490	.98347	.12079
	$3d^2$.03308	-.11737	.99254

1d

New	Old	$3s\ 3d$	$3p^2$	$3d^2$
	$3s3d$.89843	.43093	-.01285
	$3p^2$	-.43732	.89702	.06405
	$3d^2$.39642	-.05193	.99786

3p

New	Old	$3p^2$	$3d^2$
	$3p^2$.99884	.04807
	$3d^2$	-.04807	.99884

TABLE D-7
THE UNITARY MATRICES $|\langle \psi_1 | \psi_2 \rangle|, (1^2 2^6 3^2)^o$

1_R			3_R		
Now	Old	3s3p	Now	Old	3s3p
3s3p		.99168	3s3p		.99877
3p3d		-.12875	3p3d		-.04956

TABLE D-8
THE UNITARY MATRICES $|\langle \text{arf} | \text{tr} \rangle|$ $1^2 2^8 3^{16}$

1_s

New \ Old	$3p^6 3d^{10}$	$3s^2 3p^4 3d^{10}$	$3s^2 3p^6 3d^8$
$3p^6 3d^{10}$.99491	-.09904	.01833
$3s^2 3p^4 3d^{10}$.09991	.99345	.05552
$3s^2 3p^6 3d^8$	-.01271	.05707	.99829

1_d

New \ Old	$3s3p^6 3d^9$	$3s^2 3p^4 3d^{10}$	$3s^2 3p^6 3d^8$
$3s3p^6 3d^9$.831773	.555116	.000637
$3s^2 3p^9 3d^{10}$	-.554800	.831337	-.032791
$3s^2 3p^6 3d^8$	-.018733	.026921	.999462

3_p

New \ Old	$3s^2 3p^4 3d^{10}$	$3s^2 3p^6 3d^8$
$3s^2 3p^4 3d^{10}$.999707	-.024220
$3s^2 3p^6 3d^8$.024220	.999707

TABLE D-9
THE UNITARY MATRICES $|\langle \text{arr} | \text{tr} \rangle|, (1^2 2^8 3^{16})^0$

$1p^0$

New \ Old	$3s 3p^5 3d^{10}$	$3s^2 3p^5 3d^9$
$3s 3p^5 3d^{10}$.99770	-.06782
$3s^2 3p^5 3d^9$.06782	.99770

$3p^0$

New \ Old	$3s 3p^5 3d^{10}$	$3s^2 3p^5 3d^9$
$3s 3p^5 3d^{10}$.99960	-.02818
$3s^2 3p^5 3d^9$.02818	.99960

We call attention to the following features of the results.

(i) In the complexes considered here, the effects of configuration mixing within a given complex are comparable in magnitude with the corresponding effects in complexes of the form $(l^2 2^q)$ studied previously. Thus, the mixing coefficients, which indicate the magnitude of departures from the central field approximation, are of the order of .1 and the changes in the intervals ΔW_1 between adjacent terms are of the order of 10-30%.

(ii) In a few instances the changes may be much greater than the values mentioned in the last paragraph. For example, the configurations $3s3d$ and $3p^2$ in the complex $(l^2 2^8 3^2)$ are very strongly mixed, the mixing coefficients being about .44. The same is true of the corresponding pair of configurations in the complex $(l^2 2^8 3^{16})$, where the mixing coefficients are about .55. In these cases the resulting change in the value of W_1 is great enough to change the original order of the spectroscopic term (for large Z). Thus $W_1(^1D)$ actually lies below the value of $W_1(^3P)$ in the configuration $3p^2$ of $(l^2 2^8 3^2)$ when allowance is made for configuration mixing within the complex. The change in W_1 for this term thus exceeds 100% of the separation $\Delta W_1 = W_1(^1D) - W_1(^3P)$ as predicted by the Slater theory.

(iii) It is necessary in general to allow for all effects of configuration mixing within a given complex, though in particular cases some contributions may be negligible. In particular, interactions connecting configurations that differ in the quantum numbers of a single electron cannot in general be neglected be-

side interactions that connect configurations that differ through the quantum numbers of two electrons. The configurations $3s3d$ and $3p^2$ discussed in the last paragraph illustrate this point.

(iv) The effects of configuration mixing are smaller in the complex $(1^2 2^8 3^{16})$ than in $(1^2 2^8 3^2)$. This behavior is similar to that observed in complexes of the type $(1^2 2^q)$: The effects of configuration mixing tend to diminish with increasing q . The reason is that the off-diagonal elements of electrostatic interaction are essentially independent of the number of electrons in the system, whereas the differences between diagonal elements of the energy matrix increase with increasing N (total number of electrons). Since the mixing coefficients are, in a first approximation, equal to the ratios between off-diagonal interaction elements and diagonal energy differences, they will tend to diminish with increasing N .

D.3. The Semi-Empirical Method of Bacher and Goudsmit

The method of Bacher and Goudsmit (D-8) seeks to relate the term energies of an N -electron atom with the term energies of its ions, so that if the appropriate term energies of systems (M, Z) with $M < N$ are known (from either theory or experiment) one can calculate the term energies of the system (N, Z) to a certain approximation.

The theoretical relations connecting the N -electron energies with the 1-, 2-, ..., $(N - 1)$ -electron energies are based on the independent-orbital approximation. That is, each electron is assigned a definite pair of orbital quantum numbers nl . We

now derive these relations, using a more explicit notation than that of Bacher and Goudsmit.

Let q_1 denote the number of 1s orbitals, q_2 the number of 2s orbitals, q_3 the number of 2p orbitals, and so on up to q_r , so that for an N-electron atom

$$q_1 + q_2 + \dots + q_r = N .$$

Let Γ_N denote the set of quantum numbers that are required, in addition to the q_i , to specify the state of an N-electron atom.

Consider a given state $(q_i)\Gamma_N$. An M-electron subsystem, consisting of the nucleus and $M < N$ electrons, will not in general be in a definite state $(\alpha^1 \dots \alpha^M)\Gamma_M$. The α^i denote pairs of orbital quantum numbers, not necessarily all distinct, selected from the set of N pairs that characterize the N-electron state under consideration. We shall use the abbreviation $(\alpha^1 \dots \alpha^M) = \alpha_M$. Thus we may use the symbol $\alpha_M\Gamma_N$ in place of $(q_1 \dots q_r)\Gamma_N$. With every state $\alpha_M\Gamma_M$ we may associate a definite probability $P(\alpha_M\Gamma_M | \alpha_N\Gamma_N)$. More generally, we consider the set of all probabilities of the type $P(\alpha_A\Gamma_A | \alpha_B\Gamma_B)$, where $A < B < N$ and the set α_A is contained in the set α_B . These probabilities are not all independent, since they evidently satisfy all relations of the form

$$\sum_B P(\Gamma_A | \Gamma_B) P(\Gamma_B | \Gamma_C) = P(\Gamma_A | \Gamma_C) . \quad (D-1)$$

(For simplicity we have omitted the labels α .)

By means of what are now standard methods in the theory of complex spectra, one can evaluate any probability $P(\alpha_A\Gamma_A | \alpha_B\Gamma_B)$.

Let $W(\alpha_M \Gamma_M | \alpha_N \Gamma_N)$ denote the energy of the M-electron subsystem in state Γ_M , considered as part of the N-electron system in state Γ_N . Then

$$\bar{W}(\alpha_M | \alpha_N \Gamma_N) = \sum_{\Gamma_M} P(\alpha_M \Gamma_M | \alpha_N \Gamma_N) W(\alpha_M \Gamma_M | \alpha_N \Gamma_N)$$

is the mean energy associated with the subconfiguration α_M when the N-electron system is in state Γ_N . Note that the energies $W(\alpha_M \Gamma_M | \alpha_N \Gamma_N)$ do not coincide with the energies of the corresponding M-electron ions of the N-electron system which would be denoted by $W(\alpha_M \Gamma_M | \alpha_M \Gamma_M)$, because the electrons in the subsystem move in the combined field of a nuclear charge Z and N-1 orbital electrons, while the electrons in the ion move in the combined field of the same nuclear charge and M-1 orbital electrons. Thus the energy levels of the subsystem lie above the corresponding levels of the ion. However, in practical applications of the method to be described, Bacher and Goudsmit used empirical ionic energies as approximations to the corresponding subsystem energies. The latter cannot, of course, be obtained directly from experiment. We shall return to this question later.

Following Bacher and Goudsmit, we write the energy of an M-electron subsystem as a weighted sum of contributions $w(\alpha_K \Gamma_K)$, $K < M$, where α_K stands for a set of K labels $\alpha^1, \dots, \alpha^K$ selected from the set of M labels $\alpha_M = \alpha^1, \dots, \alpha^M$. The energy contributions w are defined implicitly by the set of equations

$$W(\alpha_M \Gamma_M) = \sum_{\alpha} w(\alpha) + \sum_{\alpha_2} \bar{w}(\alpha_2 | \alpha_M \Gamma_M) + \dots + \sum_{\alpha_K} \bar{w}(\alpha_K | \alpha_M \Gamma_M) + \dots + w(\alpha_M \Gamma_M) . \quad (D-2)$$

The mean energy contributions \bar{W} are defined in analogy with the mean energies \bar{W} :

$$\bar{w}(\alpha_K \Gamma_K | \alpha_M \Gamma_M) = \sum_{\Gamma_K} P(\alpha_K \Gamma_K | \alpha_M \Gamma_M) w(\alpha_K \Gamma_K) \quad (D-3)$$

The set of all these equations, for all states $\alpha_M \Gamma_M$ with $M < N$, has a unique solution for the energy contributions w in terms of the energies W :

$$\begin{aligned} w(\alpha_M \Gamma_M) &= W(\alpha_M \Gamma_M) - \sum_{\alpha_{M-1}} \bar{W}(\alpha_{M-1} | \alpha_M \Gamma_M) + \sum_{\alpha_{M-2}} \bar{W}(\alpha_{M-2} | \alpha_M \Gamma_M) \\ &\quad - \dots - (-1)^M \sum_{\alpha} W(\alpha) \end{aligned} \quad (D-4)$$

In this equation all energies pertain to subsystems of the N -electron system in the state $\alpha_N \Gamma_N$. The proof of the formula is by mathematical induction. For $M = 1$, the formula reduces to

$$W(\alpha) = w(\alpha) , \quad (D-5)$$

which coincides with equation (D-2) for $M = 1$. Suppose now that the formula holds for $M = 1, \dots, n$. We now show that it must then hold for $M = n+1$. From equation (D-4) we have,

$$\begin{aligned} w(\alpha_{n+1} \Gamma_{n+1}) &= W(\alpha_{n+1} \Gamma_{n+1}) - \\ &\quad - \sum_{\alpha_n \Gamma_n} P(\alpha_n \Gamma_n | \alpha_{n+1} \Gamma_{n+1}) \times \\ &\quad \times [W(\alpha_n \Gamma_n) - \sum_{\alpha_{n-1} \Gamma_{n-1}} P(\alpha_{n-1} \Gamma_{n-1} | \alpha_n \Gamma_n) W(\alpha_{n-1} \Gamma_{n-1}) + \dots] - \end{aligned}$$

$$\begin{aligned}
& - \sum_{\alpha_{n-1} \Gamma_{n-1}} P(\alpha_{n-1} \Gamma_{n-1} | \alpha_{n+1} \Gamma_{n+1}) \times \\
& \times [W(\alpha_{n-1} \Gamma_{n-1}) - \sum_{\alpha_{n-2} \Gamma_{n-2}} P(\alpha_{n-2} \Gamma_{n-2} | \alpha_n \Gamma_n) W(\alpha_{n-2} \Gamma_{n-2}) + \dots] \dots
\end{aligned} \tag{D-6}$$

Using the probability-composition rule (D-1), we can put the right side of this relation into the form

$$W(\alpha_{n+1} \Gamma_{n+1}) + \sum_{k=1}^n c_k \sum_{\alpha_{n+1-k}} \bar{W}(\alpha_{n+1-k} | \alpha_{n+1} \Gamma_{n+1}) . \tag{D-7}$$

The number of individual contributions to the k th summand is $c_k \binom{n+1}{k}$. This number is also given by

$$\sum_{j=0}^k (-1)^j \binom{n+1-j}{n-k} \binom{n+1}{n+1-j} = (-1)^k \binom{n+1}{n-k} + \sum_{j=0}^{k+1} (-1)^j \binom{n+1-j}{n-k} \binom{n+1}{n+1-j} . \tag{D-8}$$

Using the addition theorem for binomial coefficients, we obtain

$$\sum_{j=0}^{k+1} (-1)^j \binom{n+1-j}{n-k} \binom{n+1}{n+1-j} = (-1)^{k+1} \binom{0}{k+1} = 0 . \tag{D-9}$$

Hence

$$c_k = (-1)^k , \tag{-10}$$

which completes the proof.

Bacher and Goudsmit assume that, for a given state $\alpha_N \Gamma_N$, the energy contributions

$$\sum w(\alpha_k | \alpha_N \Gamma_N)$$

diminish rapidly with k . Consider the expansion

$$W(a_N \Gamma_N) = \sum_a W(a) + \sum_{a_2} \bar{W}(a_2 | a_N \Gamma_N) + \dots + \sum_{a_k} \bar{W}(a_k | a_N \Gamma_N) + \dots + W(a_N \Gamma_N) , \quad (D-11)$$

which is a special case of equation (D-2). By omitting the last term on the right we obtain an approximate formula for the energy of the N -electron system in terms of quantities pertaining to k -electron subsystems with $k \leq N$. From equation (D-4) it follows that the approximation $W(a_N \Gamma_N) = 0$ is equivalent to the approximation

$$W(a_N \Gamma_N) = \sum_{a_{N-1}} \bar{W}(a_{N-1} | a_N \Gamma_N) - \sum_{a_{N-2}} \bar{W}(a_{N-2} | a_N \Gamma_N) + \dots + \sum_a \bar{W}(a | a_N \Gamma_N) . \quad (D-12)$$

Thus the energy of the N -electron system is expressed as a linear combination of energies of k -electron subsystems with $k < N$.

More generally, we obtain the k th approximation in the sense of Bacher and Goudsmit when we retain the first $k+1$ terms on the right side of equation (D-11). In particular, the first approximation (which is exact for 2-electron systems) is defined by the equation

$$W^{(1)}(a_N \Gamma_N) = \sum_a W(a) + \sum_{a_2} \bar{W}(a_2 | a_N \Gamma_N) .$$

$$= \sum_{a_2} \bar{W}(a_2 | a_N \Gamma_N) - (N-2) \sum_a W(a | a_N \Gamma_N) . \quad (D-13)$$

With the help of equation (D-4) we can express $W^{(k)}$, for any $k < N$, as a linear combination of energies pertaining to $(k+1)$ -electron subsystems.

In practical applications of the Bacher-Goudsmit approximation method one uses experimental values of the ionic energies $W(\alpha_k \Gamma_k | \alpha_k \Gamma_k)$ in place of the subsystem energies $W(\alpha_k \Gamma_k | \alpha_N \Gamma_N)$. In order for this to be a good approximation, the electrons that are present in the N -electron system but not in the k -electron subsystem must make only a minor contribution to the electrostatic field seen by the remaining electrons. Since the removal of "core electrons" (electrons in closed shells) does substantially alter the effective electrostatic field of the atom, one should always regard the core electrons and the field they produce as fixed. That is, one should reckon all energies from the core energy as a fixed zero-point. The formulae already developed apply without change to these relative energies, since they do not depend on any assumptions regarding the nuclear contribution to the electrostatic field except the assumption of radial symmetry. Since the core, by definition, is composed of complete groups of electrons, its contribution to the field will have spherical symmetry and may therefore be lumped with the nuclear contribution.

D.4. The Bacher-Goudsmit Method and Configuration Mixing

The independent-orbital approximation is just as basic in the theory of Bacher and Goudsmit as in the theory of Slater. The basic equations of the theory, (D-2) and (D-4),

presuppose the possibility of assigning every subsystem of an N -electron system to a definite electronic configuration, and the coefficients in these equations are to be evaluated by means of a theory based on the same approximation. Nevertheless, the Bacher-Goudsmit approximation does, in a sense, allow for certain effects of configuration mixing, because it makes use of empirical ionic energies. Since these include contributions from configuration mixing, so must the "predicted" energies. Now, the approximation of greatest practical and theoretical interest in the Bacher-Goudsmit scheme is the first one, which yields the energies $W^{(1)}$ defined by equation (B-13). The question therefore arises: Which effects of configuration mixing are included in $W^{(1)}$ when the two-electron energies $w(a_2 \Gamma_2 | a_N \Gamma_N)$ are taken from experiment?

Bacher and Goudsmit discuss this question briefly and schematically, using ordinary perturbation theory. They conclude (incorrectly, as we shall see) that the first approximation includes all effects of configuration mixing with doubly excited configurations (i.e., configurations differing from the original one in two pairs of one-electron quantum numbers). They also conclude (correctly) that the first approximation does not include all effects of configuration mixing with singly excited configurations. Before turning to a detailed consideration of these questions, however, let us examine the problem from another angle.

As has previously been pointed out (Layzer^(B-1)), the Slater theory predicts certain qualitative regularities in the structure of term spectra, which do not accord with the

observed regularities. For example, the Slater theory predicts that all configurations consisting of n or $6-n$ equivalent p electrons, together with any number of complete groups, have the same structure apart from a scale factor. Specifically, if $n = 2, 3$, or 4 , the two independent intervals between the spectroscopic terms with $L = 0, 1, 2$ are predicted to satisfy the relation $SD/DP = 3/2$. The Z -dependent approximation scheme predicts different qualitative and quantitative regularities. It predicts, for example, that the interval ratio SD/DP approaches a constant value with increasing Z in a given isoelectronic sequence, and that this constant (which can be calculated from the theory) depends both on the principal quantum numbers of the p electrons and on the complete groups present in the electronic configuration. How does the Bacher-Goudsmit theory stand on this matter?

Consider a simple example, the configuration $1s^2 2s^2 2p^2$ in the carbon sequence. We regard the K -electrons as composing a fixed core, and proceed to calculate the term energies relative to this core in the approximation (D-13). We obtain

$$W^{(1)}(2s^2 2p^2 SL) = W(2s^2) + \bar{W}(2s2p) + W(2p^2 SL) - 4W(2s) - 4W(2p), \quad (D-14)$$

where we have omitted unnecessary labels on the right side. Note that the mean two-electron energy $\bar{W}(2s2p)$ does not depend on the quantum numbers SL , because the two $2s$ electrons form a complete group. From this equation we see at once that the configuration $2s^2 2p^2$ is predicted to have the same structure as the configuration $2p^2$. Actually, the interval ratio SD/DP

is substantially less than 3/2 in all systems belonging to the beryllium sequence (i.e., in all configurations $1s^2 2p^2$). The difference between the two limiting ratios is due to the mixing of configurations belonging to the same complex; both limiting ratios are correctly predicted by the Z-dependent theory. We conclude, therefore, that the Bacher-Goudsmit method does not in general allow correctly for this type of configuration mixing -- the most important type according to the Z-dependent theory -- in the first approximation.

Now, in the example just given the "perturbing" configurations that need to be considered if the limiting interval ratios are to be correctly predicted are $2p^4$ (interacting with $2s^2 2p^2$) and $2s^2$ (interacting with $2p^2$). These are "doubly excited" configurations in the sense explained above (though the configuration $2s^2$ should perhaps be described as doubly de-excited relative to $2p^2$). It follows that the first approximation in the Bacher-Goudsmit scheme does not, in fact, allow fully for the effects of mixing with doubly excited configurations.

The argument given by Bacher and Goudsmit fails because it does not allow properly for the Pauli exclusion principle. Bacher and Goudsmit tacitly assume a strict correspondence between doubly excited N-electron configurations and doubly excited configurations in which the principal quantum numbers of the excited electrons differ from those of the original electrons. It does not, however, extend to doubly excited configurations with the same principal quantum numbers as the original configuration. Thus, the de-excitation

of the 2p electrons in the configuration $2p^2$ to form the configuration $2s^2$ is permitted by the exclusion principle; but in the configuration $2s^2 2p^2$, de-excitation of the 2p electrons would yield the non-permitted configuration $2s^4$.

The predictions of the first-order Bacher-Goudsmit theory differ from those of the first-order Z-dependent theory in other important respects. For example, we have seen (see subsection 2) that the effects of mixing with singly excited configurations may be very large. We have also seen that in some instances the effects of configuration mixing are too large to be adequately described by second-order perturbation theory. Finally, we have seen that the effects of configuration mixing are systematically greater in almost-empty shells than in the corresponding almost-full shells. All these features of the Z-dependent theory are at variance with the first-order Bacher-Goudsmit theory.

We conclude that the Bacher-Goudsmit theory does not provide a satisfactory framework for dealing with the most important effects of configuration mixing, even semi-empirically.

D.5. The Modified Slater Theory

The theory of Bacher and Goudsmit is held by Racah (D-7) to provide a theoretical justification for the $L(L + 1)$ correction in the following sense. By means of equation (D-13) one can express the energies of an N-elec-

tron system in terms of the energies of two-electron systems. Let us admit, for the sake of the argument, that the dominant effects of configuration mixing for the N -electron system are included in the energies calculated with equation (D-13) if one uses the true values of the energies $W(\alpha_2 \Gamma_2 | \alpha_N \Gamma_N)$ in evaluating the right side. Instead of using experimental values for the last-named energies, one could use an interpolation formula containing a number of adjustable parameters. Suppose we are considering configurations of the type d^n . The configuration d^2 has five terms, so that if one uses an interpolation formula with five adjustable parameters, the values of the parameters will be uniquely determined by experiment. Equation (D-13) then enables one to express the energy of any term belonging to the configuration d^n in terms of these five parameters.* According to Slater's theory, the mean energy of all the terms in a given configuration labelled by given values of S and L is a linear combination of certain radial integrals, the Slater F and G integrals. For configurations d^n there are three such integrals: F^0 , F^2 and F^4 . However, even if one regards these as adjustable parameters, one cannot obtain a very good representation of the experimental data. The addition of two empirical correction terms, $\alpha L(L + 1) + \beta Q$, the second

*In practice the parameters are not regarded as having fixed values, corresponding to the configuration d^2 , but as functions of the effective central field. One can evaluate the parameters for $n > 2$ by equating the predicted energies to their experimental counterparts and solving the resulting equations by the method of least-squares.

of which was suggested by Racah^(D-6), makes it possible to represent the term energies in the configuration d^2 exactly and to represent the term energies in other configurations that have been examined with fairly good accuracy.

From the discussion in the preceding subsections, however, we know that equation (D-13) does not provide a satisfactory framework for dealing with the dominant effects of configuration mixing. It is true that the empirical description of spectra in the iron group based on the Slater-Racah interpolation formulae has been remarkably successful. However, guided by the considerations of the present paper, one can easily choose examples of configurations for which the method will give poor results. A simple example is the configuration $1s^2 2s^2 2p^6 3p^2$.

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APPENDIX E
D. Layzer

RELATIVISTIC EFFECTS IN HEAVY ATOMS

E.1 Introduction

In heavy, as in light, atoms the chief groupings of energy levels have their source in the nonrelativistic (electrostatic) interactions between the electrons. These groupings are characterized by sets of principal quantum numbers (n^1). Adjacent groups are separated by intervals of the order of $Z_e^2 \alpha^2 mc^2$, where Z_e is the effective nuclear charge for the outermost electrons.

The structure of a given group, however, has an entirely different character in heavy atoms and in light atoms. In the latter, each group (or complex) splits up into spectroscopic terms consisting of levels, distinguished by the quantum number J . The spacing between terms is of the order of $Z_e^2 \alpha^2 mc^2$, while the spacing between levels in a given term is of the order of $Z_e^4 \alpha^4 mc^2$. In light atoms, by definition, $\alpha^2 Z_e^3 \ll 1$, so that the fine structure is clearly differentiated from the coarse structure. The fine structure originates in relativistic interactions between the orbital electrons and the nucleus, the coarse structure in nonrelativistic interactions between the electrons.

In heavy atoms, on the other hand, the coupling parameter $\alpha^2 Z_e^3$ is not small. Consequently the relativistic interactions cannot adequately be treated by first-order perturbation theory, as they can be in light atoms. The structure for the major groupings (complexes) is correspondingly

complicated. In general, there is no clear-cut distinction between coarse structure and fine structure; the two kinds of interactions contribute comparably to the spacing between levels in a given complex.

When $z_e^3 \alpha^2 \gg 1$, the relativistic contributions become dominant; the complex breaks up into sub complexes, characterized by quantum numbers $(n^i j^i)$. Within a given sub complex the spacing of levels is due primarily to the nonrelativistic (electrostatic) interaction.

This state of affairs is characteristic of x-ray spectra. Here z_e may be comparable to Z itself because the missing electrons belong to inner shells.

The conventional method for describing the structure of energy spectra in the intermediate-coupling regime ($\alpha^2 z_e^3 \ll 1$) is set forth in Theory of Atomic Spectra.^(E-1) It is based on the central-field approximation and allows for the leading relativistic contribution to the energy - the spin-orbit interaction. This is evaluated for electrons moving, not in the Coulomb field due to the nuclear charge Z , but in an effective central field due to the nuclear charge plus the electrons.

The conventional method has several drawbacks.

It is better suited to a semi-empirical description than a purely theoretical one. This is because the radial integrals (ξ) that determine the magnitude of the spin-orbit interaction cannot be accurately evaluated by purely theoretical means. They are best evaluated by treating them as adjustable parameters, to be assigned

values that will make the theoretical formulae fit the data as well as possible. This is nearly always the adopted in practice.

The spin-orbit interaction appears as a separate term in the Hamiltonian for a many-electron atom only in the Pauli (low Z) approximation. When Z is not small, it is by no means clear that the spin-orbit interaction adequately approximates to the relativistic part of the Hamiltonian.

An alternative description of relativistic effects in the structure and spectra of many-electron atoms is provided by recent work of Layzer and Bahcall^(E-2). This is an extension of the nonrelativistic Z -dependent theory^(E-3). The principal features of the Z -dependent relativistic theory are as follows:

(a) The Hamiltonian employed is shown to contain all known relativistic interactions up to (but not including) those of order $\alpha^4 Z^2 mc^2$. The largest known interactions not included in the Hamiltonian are those responsible for the lamb shift.

(b) The spin-orbit interaction is allowed for exactly, in the zeroth approximation - just as in the Dirac theory of the hydrogen atom.

(c) The theory enables one to evaluate all contributions of order Z^{-1} compared with the spin-orbit interaction. This is not possible with the conventional theory - and herein lies the crucial difference between the old and the new methods. It is the possibility of precisely evaluating the next-to-the-leading relativistic contributions

that renders the new method quantitative where the old one was merely semi-quantitative.

Although the next-to-the leading relativistic contributions can be evaluated in principle, the actual calculations are long and difficult. Even for such comparatively simple electronic configurations as $1s^2 2s$ and $1s^2 3s$, considered by Layzer and Bahcall^(E-2), the evaluation of these terms required a long calculation. For heavy atoms the corresponding calculations are at present prohibitively difficult. It is therefore of interest to inquire whether there is an approximation that will enable one to estimate the contributions in question with fair accuracy. We deal with this question in Section E.2. In Section E.2, we consider a related problem (as it turns out to be)-the relativistic generalization of the nonrelativistic screening parameters defined by Layzer^(E-3).

E.2 Approximate Form of the Relativistic Corrections for Heavy Atoms

The coefficient of $\alpha^2 Z^4 mc^2$ in the expression for the energy of an atomic state, according to the theory of Layzer and Bahcall^(E-2), is a function of the coupling parameter $x = \alpha^2 Z^3$. In the extreme relativistic case, this coefficient, which we denote by a_4 , is given by a direct generalization of Sommerfeld's formula:

$$a_4(x) \rightarrow \sum_{l=1}^{N_e} \frac{1}{\frac{1}{4} - \frac{n_l}{j_l}} \left(\frac{n_l}{j_l + \frac{1}{2}} - \frac{3}{4} \right) \quad \text{as } x \rightarrow \infty \quad (E-1)$$

In the opposite limit ($x \rightarrow 0$) a_4 does not approach the value that would be predicted on the basis of the central-field approximation; to obtain the correct limiting value, one must allow for the effects of configuration

mixing. (This can be done most simply by using, in place of the central-field wave function ψ , a finite linear combination of wave functions $\sum a_i \psi_i$, the constants a_i being given by the screening theory; see Appendix C.)

In the general case $a_4(x)$ can be calculated, without excessive labor, to any desired accuracy by methods described in the paper by Layzer and Bahcall cited earlier. We may, therefore, consider it to be known.

It is the coefficient $a_3(x)$ of the term $\alpha^4 Z^3 mc^2$ that presents the real problem, and which we would like to approximate.

Now in the standard theory of one-electron spectra (including x-ray spectra), the relativistic contribution to the energy is usually written in the form

$$a_4(z - \sigma)^4 \alpha^4 mc^2 + O(\alpha^6 z^6) \quad (E-2)$$

where a_4 is given by Sommerfeld's formula,

$$a_4 = \frac{1}{-2n^4} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \quad (E-1')$$

and σ is a suitably chosen constant. Evidently

$$a_3 = -4\sigma a_4; \sigma = -\frac{a_3}{4a_4} \quad (E-3)$$

Thus a knowledge of σ is equivalent to a knowledge of a_3 .

Now some, though not all, of the contributions to a_3 can be interpreted physically in terms of screening. For example, the spin-other-

orbit interactions, which contribute to a_3 , tend to reduce the magnitude of the (true) spin-orbit interaction in much the same way as the inter-electronic electrostatic interactions reduce the magnitude of the electrostatic interactions between the nucleus and the electrons. On the other hand, such two-electron interactions as the spin-spin interaction have no one-electron counterpart. The interpretation of σ as a screening parameter is therefore an oversimplification. Nevertheless, it may furnish a useful means of estimating the value of a_3 through Equation (E-3).

The simplest assumption one can make about σ is to equate it to S , the screening parameter that figures in the screening theory. A comparison of empirical values of σ for hydrogenic spectra with theoretical values of S shows that this is a fair approximation, though not as good as one might wish.

Fortunately, the fractional errors due to inaccuracies in the estimated value of σ tend to become progressively smaller with increasing Z because the quartic term becomes progressively larger in comparison with the cubic term. Thus, the screening approximation to a_3 should be considerably better for Uranium, say than for Lithium.

A semi-empirical study to improve the estimate of σ might proceed along the following lines:

The two-electron screening parameter $S(\alpha/\beta)$ [representing the screening of an α electron by a β electron] is given in a first approximation by the formula^(E-3)

$$S(\alpha/\beta) = \frac{\int_0^{\infty} \frac{P_{\alpha}^2(r)}{r} dr}{\int_0^{\infty} \frac{P_{\alpha}^2(r)}{r} dr} \int_0^{\infty} P_{\beta}^2(r^1) dr^1 \quad (E-4)$$

This can be written as

$$S(\alpha/\beta) = \int_0^{\infty} w(r_2) P\{r_{\beta} < r_{\alpha}\} dr_2 \quad (E-5)$$

i.e. as a certain weighted average of the probability $P\{r_{\beta} < r_{\alpha}\}$ that a β electron will be found closer to the nucleus than r_{α} , the distance of an α electron. The weight w is given by

$$w(r_{\alpha}) = P_{\alpha}^2(r_{\alpha}) r_{\alpha}^{-1} \quad (E-6)$$

This weighting factor is appropriate for electrostatic screening, but not necessarily for other kinds of screening. A more general law than (E-6) is:

$$w_k(r_{\alpha}) = P_{\alpha}^2(r_{\alpha}) r_{\alpha}^{-k} \quad (E-7)$$

It would be interesting to test whether, by an appropriate choice of k , one could arrive at a formula for σ in better agreement with experiment. [The connection between the total screening constants S_{α} and the two-electron screening parameters is discussed in the paper by Layzer (E-3) cited earlier.] In the meantime, the old definition ($S = \sigma$) can be used with a reasonable expectation of fair accuracy.

E.3 Relativistic Screening Parameters

The screening parameters that we have dealt with so far are defined by a nonrelativistic theory. The question naturally arises as to what constitutes the proper relativistic generalization of the screening parameters.

To begin with, the relativistic screening parameters must depend on the coupling parameter X as well as on Z . They must, in fact, have the form

$$S(X, Z) = S_0(X) + S_{-1}(X)Z^{-1} + O(Z^{-2}). \quad (E-8)$$

In the limit $X \rightarrow 0$, $S(X, Z) \rightarrow$ the nonrelativistic screening parameter $S(0, Z)$. The coefficients $S_i(X)$ are all bounded from above and below. In the relativistic limit $X \rightarrow \infty$,

$$S(X, Z) \rightarrow S_0(\infty) \quad (E-9)$$

since the remaining terms on the right side of (a) vanish in this limit.

It is possible to develop a detailed theory of the X -dependent screening parameters along the lines of the variational nonrelativistic theory. The main result is that the contributions to the screening parameters from electrons in closed shells are independent of X . Now the X -dependence of the screening parameters could be significant only in heavy atoms. Since most of the electrons in a heavy atom are normally found in closed shells, the amplitude of variation of the

screening parameters with X must be small, so that the nonrelativistic approximation to the screening parameters should be adequate for most practical purposes.

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- E-2. Layzer, D., and Bahcall, *Annals of Physics*, To Be Published.
- E-3. Layzer, D., *Annals of Physics* 9, 275 (1959).

STATISTICAL DESCRIPTION OF COMPLEX SPECTRA

F. 1. Mean Energies of Configurations and Complexes

In any partial description of complex energy spectra the mean energies of configurations and complexes play a central role. Even if no other information about the energy spectrum is available one can still obtain from the mean energies, with the help of Saha's equation, useful estimates for the concentrations of the various atomic and ionic species in a mixture of gases. Again, in constructing radial wavefunctions for use in the evaluation of absolute transition probabilities -- either by the screening approximation or by a more refined method -- one may not wish to use a different set of wavefunctions for each distinct level. In a first approximation one could then use a single set of wavefunctions corresponding to the mean energy.

If we neglect entirely the effects of configuration mixing, we can write the mean interaction energy of any configuration as a sum of two-electron contributions $\{nl, n'l'\}$. If the atom has N electrons the mean interaction energy consists of $\binom{N}{2} = N(N - 1)/2$ such contributions. For example, the mean energy of the configuration $1s^2 2s^2 2p^5$ is

$$\{1s1s\} + \{2s2s\} + 10\{2p2p\} + 4\{1s2s\} + 10\{1s2p\} + 10\{2s2p\} . \quad (F-1)$$

Here $N = 9$ and the number of two-electron interactions is $9 \times 8/2 = 36$.

The two-electron interactions can be expressed in terms of the Slater F and G integrals. The appropriate formulae are

given by Layzer (F-1) and Slater (F-2), but are implicit in earlier work by Condon and Shortley (F-3) and Shortley (F-4).

To calculate the total mean energy of a configuration, including the one-electron part, we may conveniently employ the Z -dependent screening theory. The mean energy is then given by the formula

$$\bar{W} = - \sum z_{nl}^2 q_{nl} / 2n^2 . \quad (F-2)$$

Here q_{nl} is the number of electrons of the type nl in the configuration under consideration and

$$z_{nl} = Z - s_{nl} . \quad (F-3)$$

The screening parameters s_{nl} are defined in terms of the two-electron interaction energies:

$$s_{nl} = \sum_{n'l'} (q_{n'l'} - \delta_{nl,n'l'}) s(nl|n'l') , \quad (F-4)$$

$$s(nl|n'l') = \begin{cases} \frac{n^2}{2} \frac{\partial (nl, n'l')}{\partial z_{nl}} & (nl \neq n'l') \\ \frac{1}{2} n^2 \frac{\partial (nl, nl)}{\partial z_{nl}} & (nl = n'l') \end{cases} . \quad (F-5)$$

The two-electron screening parameters depend on Z , approaching constancy as $Z \rightarrow \infty$.

The preceding discussion can easily be extended to complexes. The advantage of doing this is that the resulting formula for the mean energy of a complex will have the correct linear dependence on Z . On the other hand, if one is dealing with a complex that contains a large number of configurations, the extra work required to allow properly for all the interactions may offset the resultant gain in accuracy.

F.2. The Coefficients W_1 for Complex Configurations

Instead of working with the energies themselves, one may wish to consider the statistical properties of the energy coefficients W_1 , defined as the coefficient of Z in an expansion of the energy in powers of Z^{-1} . In this subsection we discuss briefly some relevant properties of the W_1 , before returning, in the following subsection, to the main stream of our discussion. The considerations of the subsequent subsections will apply equally to the energies themselves and to the coefficients W_1 .

The coefficient W_1 is composed of two parts. The two-electron part \bar{W}_1 can be calculated from the two-electron interactions and is the same for all levels belonging to a given configuration. The remainder of W_1 , which we denote by W'_1 , results partly from LS-dependent interactions within the configuration and partly from interactions connecting terms belonging to different configurations in the same complex. It has been shown (Layzer ^(F-1)) that in atoms with a

partly-filled L shell these two contributions to W_1' are often comparable in magnitude. Some recent, as yet unpublished, calculations show that the same is true of atoms with partly-filled M shells. Hence the effects of configuration mixing within a complex cannot in general be neglected beside the LS-dependent contributions from interactions within a given configuration.

As a preliminary to calculations of W_1' that allow properly for the effects of configuration mixing, and as a temporary substitute for such calculations, we may conveniently evaluate the contributions to W_1' from interactions within the configuration. This is by no means a trivial matter for complex configurations, since such configurations may contain several distinct spectroscopic terms characterized by given values of S and L. In the representations normally used the energy operator is diagonal with respect to S and L but not with respect to the quantum numbers that serve to distinguish spectroscopic terms with the same S and L. Hence the energy matrix, instead of being diagonal, will in general consist of multi-dimensional blocks. This is the form in which energy calculations have usually been left in the past. In order to complete the diagonalization one needs to know the ratios of the various Slater integrals that figure in the energy matrix elements. In the standard theory of complex spectra these ratios are regarded either as parameters to be determined semi-empirically, or as theoretical quantities whose evaluation requires the solution of a set of Hartree-Fock equations. On the other hand, in the Z-dependent scheme one evaluates the Slater integrals using straight hydrogenic wavefunctions. The contributions to W_1' from interactions within a given configuration have definite numerical values.

which can be calculated once and for all, as can the elements of the transformation matrices that diagonalize the blocks referring to spectroscopic terms of given S and L . The transformation to a representation in which W_1 has no nondiagonal elements connecting terms in the same configuration is the first step toward the ultimate objective of a representation in which the energy matrix has no nondiagonal elements connecting terms belonging to the same complex.

F.3. The Variance of the Energy

The variance of the energy (in a given configuration) is defined by

$$\text{var } W = \langle (W - \bar{W})^2 \rangle \equiv \sigma_w^2. \quad (F-6)$$

Moszkowski (F-5) has written down formulae that give σ_w for an arbitrarily complex configuration in terms of the σ_w 's for two-electron configurations. The latter can easily be evaluated by direct calculation. Proofs of Moszkowski's formulae have not as yet appeared; but for the purposes of this report we shall assume that the formulae are correct -- or at least that σ_w can be found for any configuration of interest.

The parameter σ_w measures, roughly, the width of a configuration. Knowing σ_w , one can estimate (from Boltzmann's formula) the variation in the population of levels over a given configuration. More generally, one can estimate the error that results, in any particular calculation, from assigning the same energy to all levels in a given configuration. From σ_w one can also derive a rough estimate for

the average spacing between levels in a configuration. Thus if one assumes that, say, 50% of the levels lie in the range $W \pm \sigma_w$, one can reasonably expect the resulting estimate of the level spacing to be accurate to within a factor of 2.

F.4. The Distribution Function of the Levels in a Configuration

Knowing σ we know the width of the probability distribution, but not its shape. The question now arises: What is the best assumption as to the shape of the distribution that is consistent with our limited knowledge of the energy spectrum?

In addition to \bar{W} and σ_w we know from direct calculations that the distribution of energy levels in a configuration is strongly skewed. This fact has suggested (unpublished Convair report, 1961) that the distribution can be represented by an exponential function of the energy. Once the exponential form has been chosen, the two parameters on which such a distribution depends are uniquely determined by the values of \bar{W} and σ_w . In fact, the distribution is given by

$$p(W) = \begin{cases} N \exp [-(W - \bar{W})/\sigma_w] & (W > \bar{W} - \sigma_w) \\ 0 & (W < \bar{W} - \sigma_w) \end{cases} \quad (F-7)$$

Thus the energy spectrum is supposed to have a sharp cut-off σ_w units below the mean energy \bar{W} . The probability distribution achieves its maximum value at the cut-off and then falls off exponentially.

Before this law, or any such law, can be compared with experiment we need to have some reasonable and consistent way of passing from the theoretical or experimental energy spectrum, which is discrete, to a continuous probability distribution. One such way is the following. We assign to each level the appropriate statistical weight $(2S + 1)$. Then we divide the energy range into a convenient number of equal intervals, bounded on the left by the lowest energy in the configuration, and determine the total statistical weight of all levels falling in each energy interval. We then plot a histogram of the running means of the statistical weights against the energy. This corresponds to smearing out the discrete energy levels, which occur in bundles, into a somewhat continuous distribution of energy. As long as the intervals used to smooth the data are reasonable small compared with the total energy range, the exact manner of smoothing is of no importance. One should bear in mind that, as discussed in Subsection F.2, the distribution of energy levels as calculated with neglect of configuration mixing is at best semi-quantitative, so that much of the detail present in an unsmoothed plot of the distribution of energy levels is spurious anyway.

Figures F-1 thru F-6 illustrate the smoothed distributions of energy levels in configurations consisting of equivalent d and f electrons. Experimental data from the compilation by Miss Moore^(F-8), are taken for the d-electron configurations and theoretical energies are taken for the f-electron configuration from the paper by Elliot, Judd and Runciman.^(F-9) If in the experimental data all theoretical terms are not identified, the missing terms are given in each figure. These plots exemplify the skewed character of energy distribution, but the skewness appears to be much less marked than that associated with the exponential

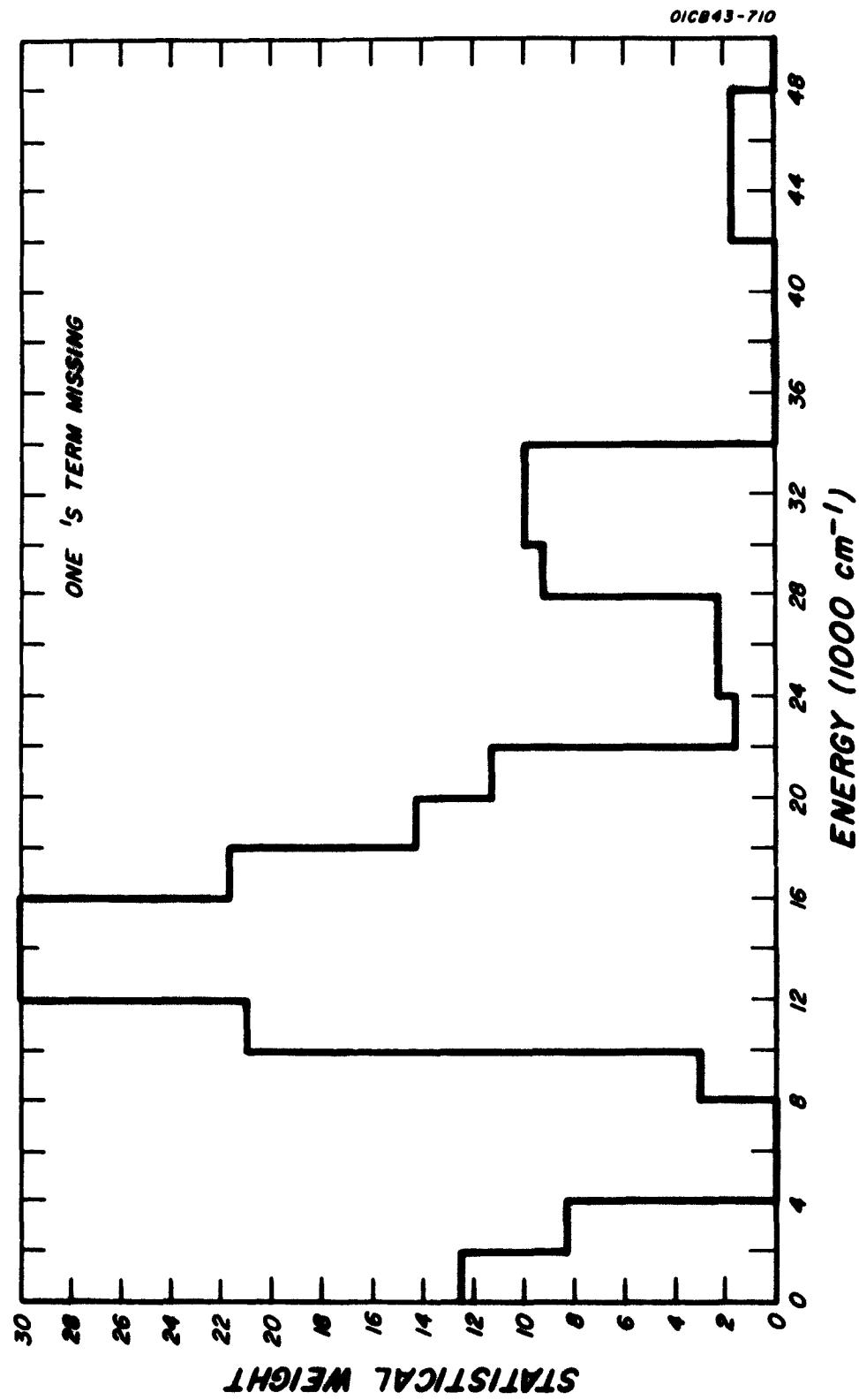


Figure F-1. Smoothed Distribution of Experimental Energy Levels in V II (Configuration $3d^4$)

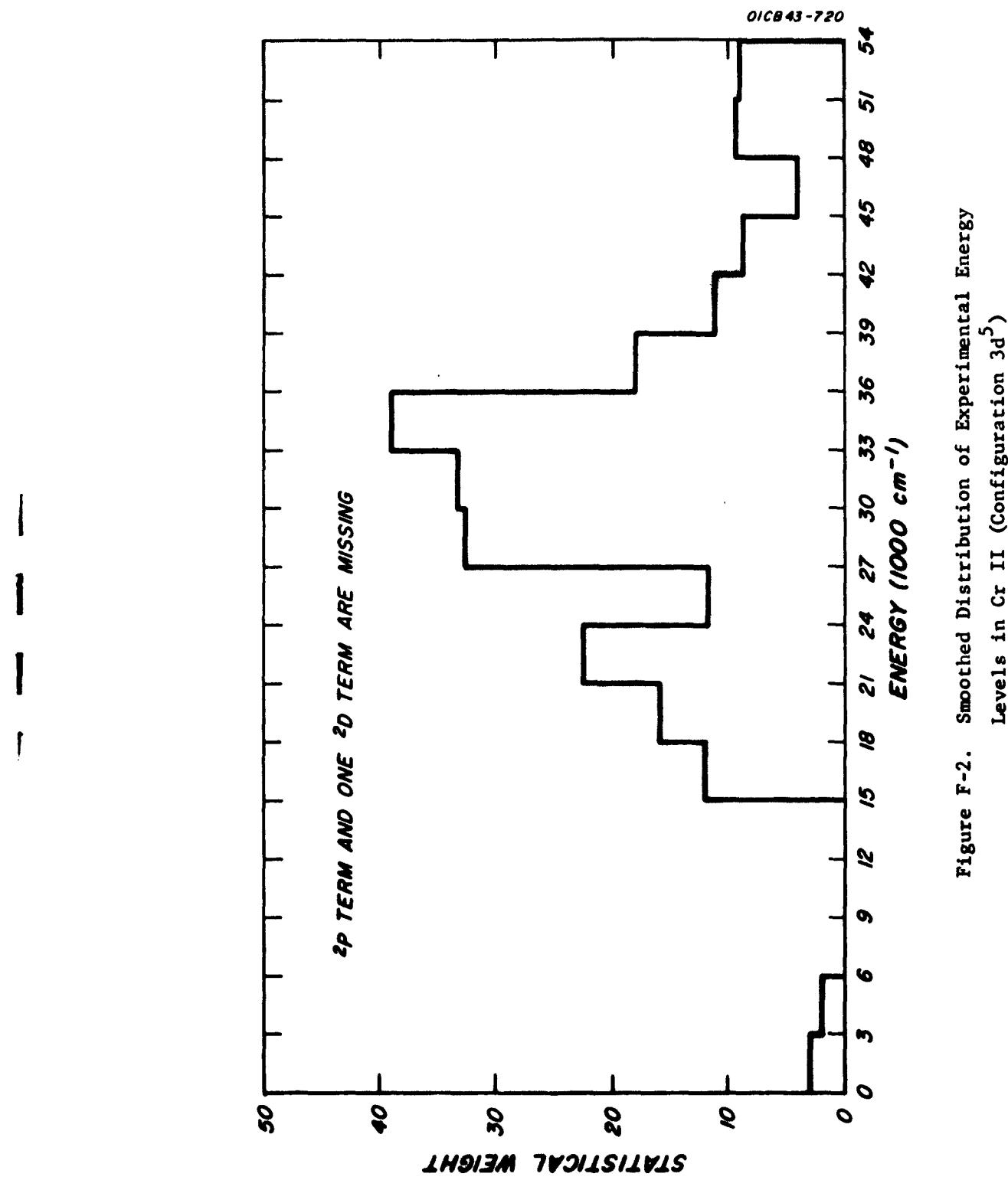


Figure F-2. Smoothed Distribution of Experimental Energy Levels in Cr II (Configuration $3d^5$)

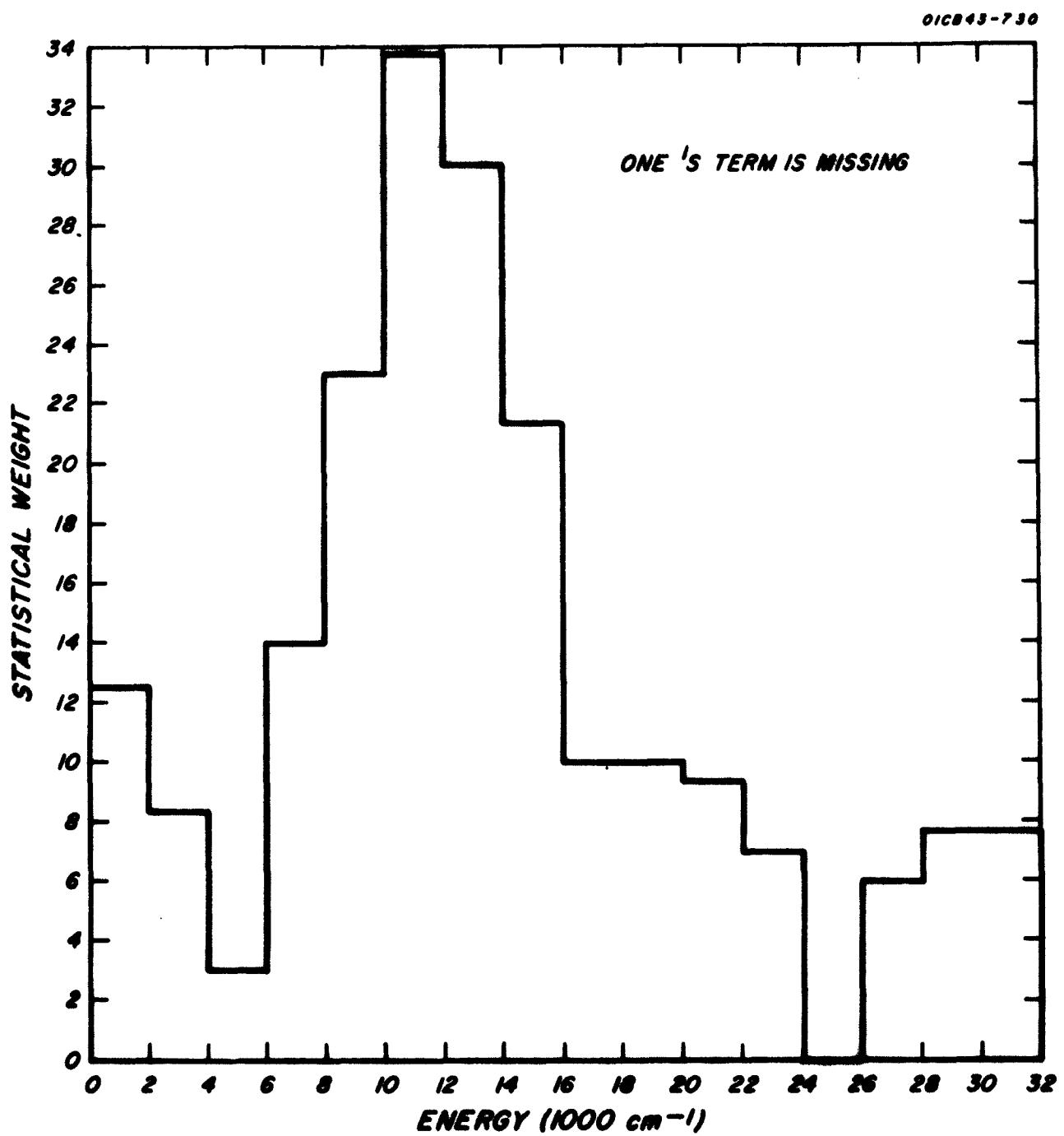


Figure F-3. Smoothed Distribution of Experimental Energy Levels in Nb II (Configuration $4d^4$).

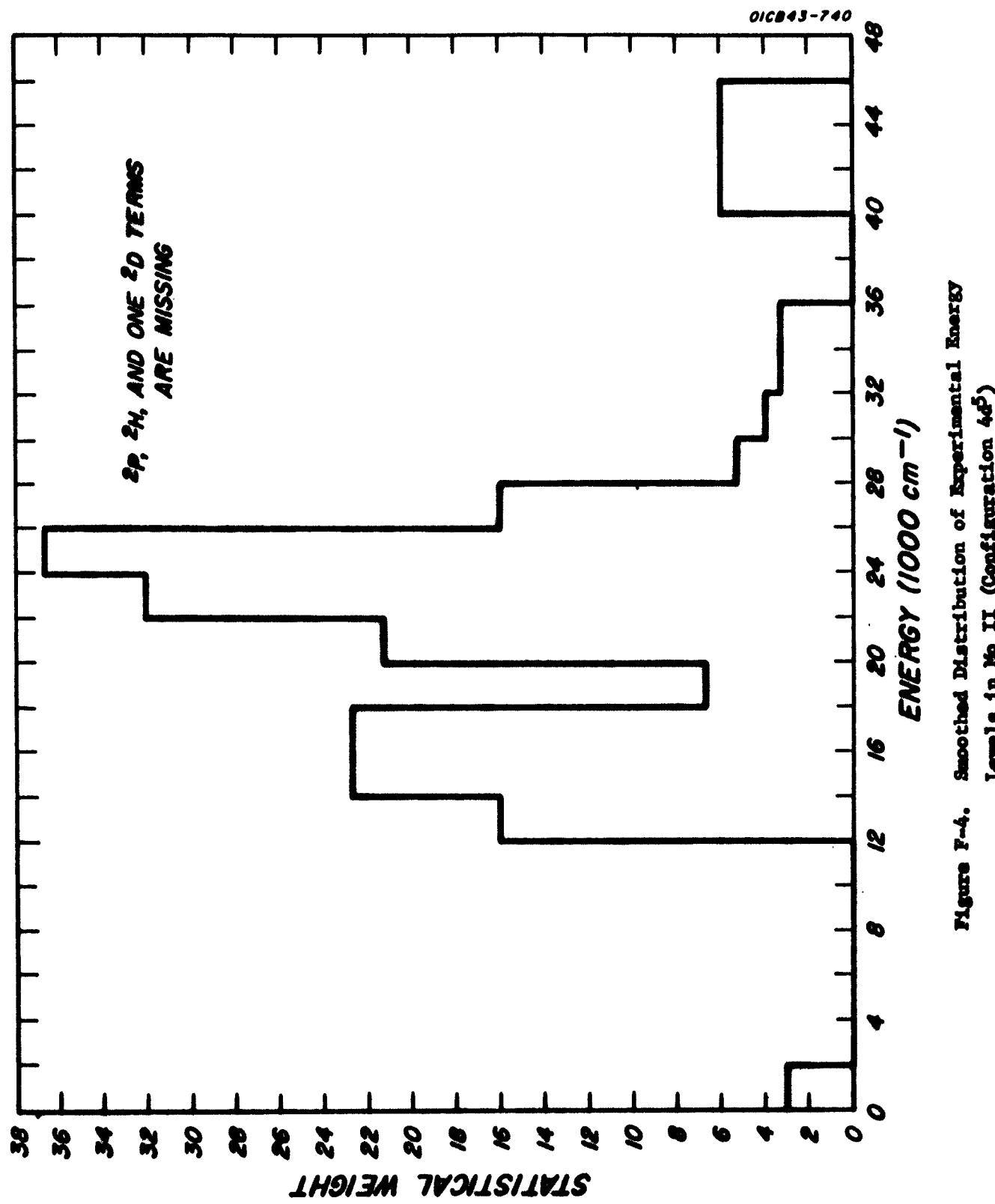


Figure Y-4. Smoothed Distribution of Experimental Energy Levels in Mo II (Configuration $4P_5$)

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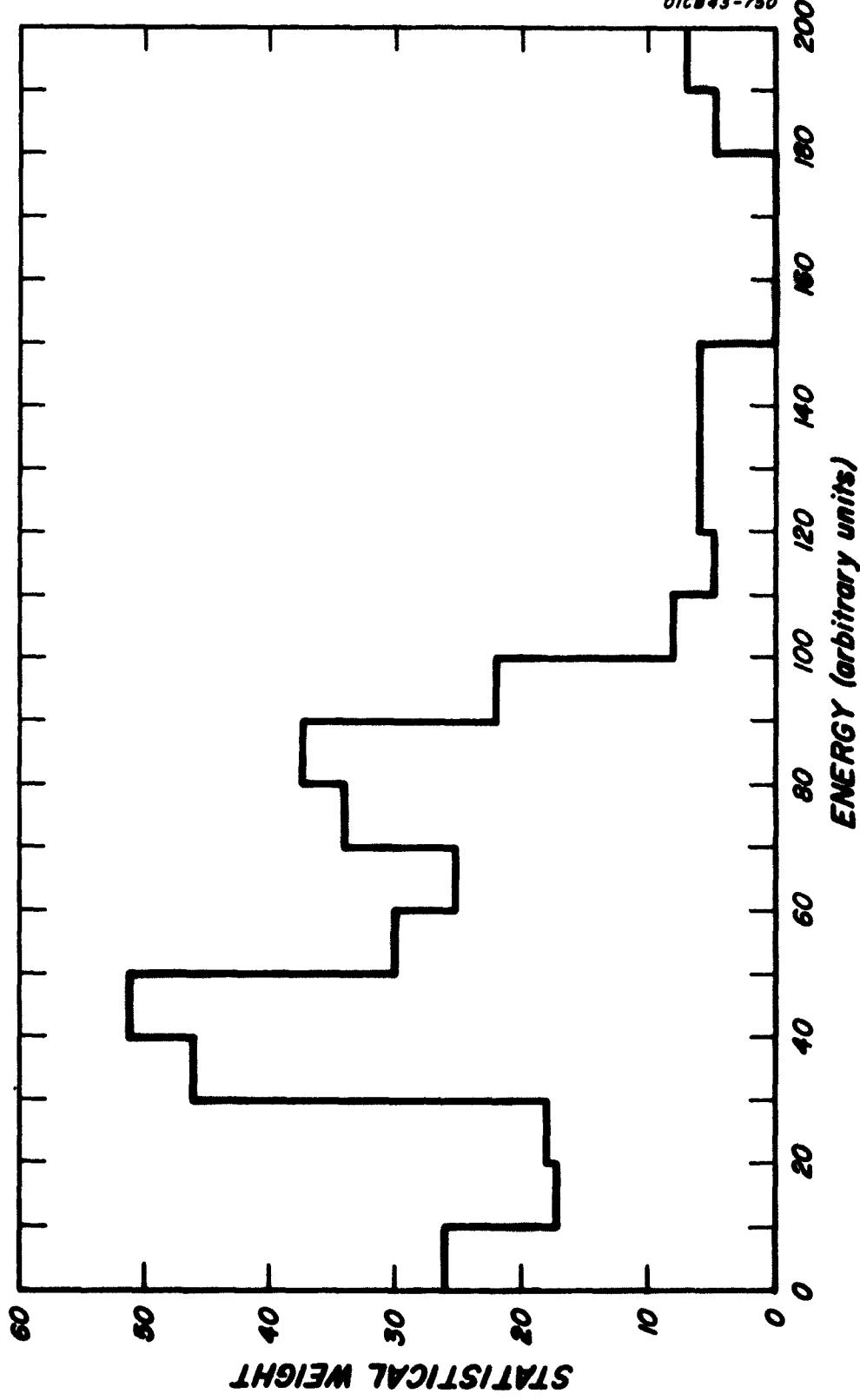


Figure F-5. Smoothed Distribution of Theoretical Energy
level in the Configuration f^3

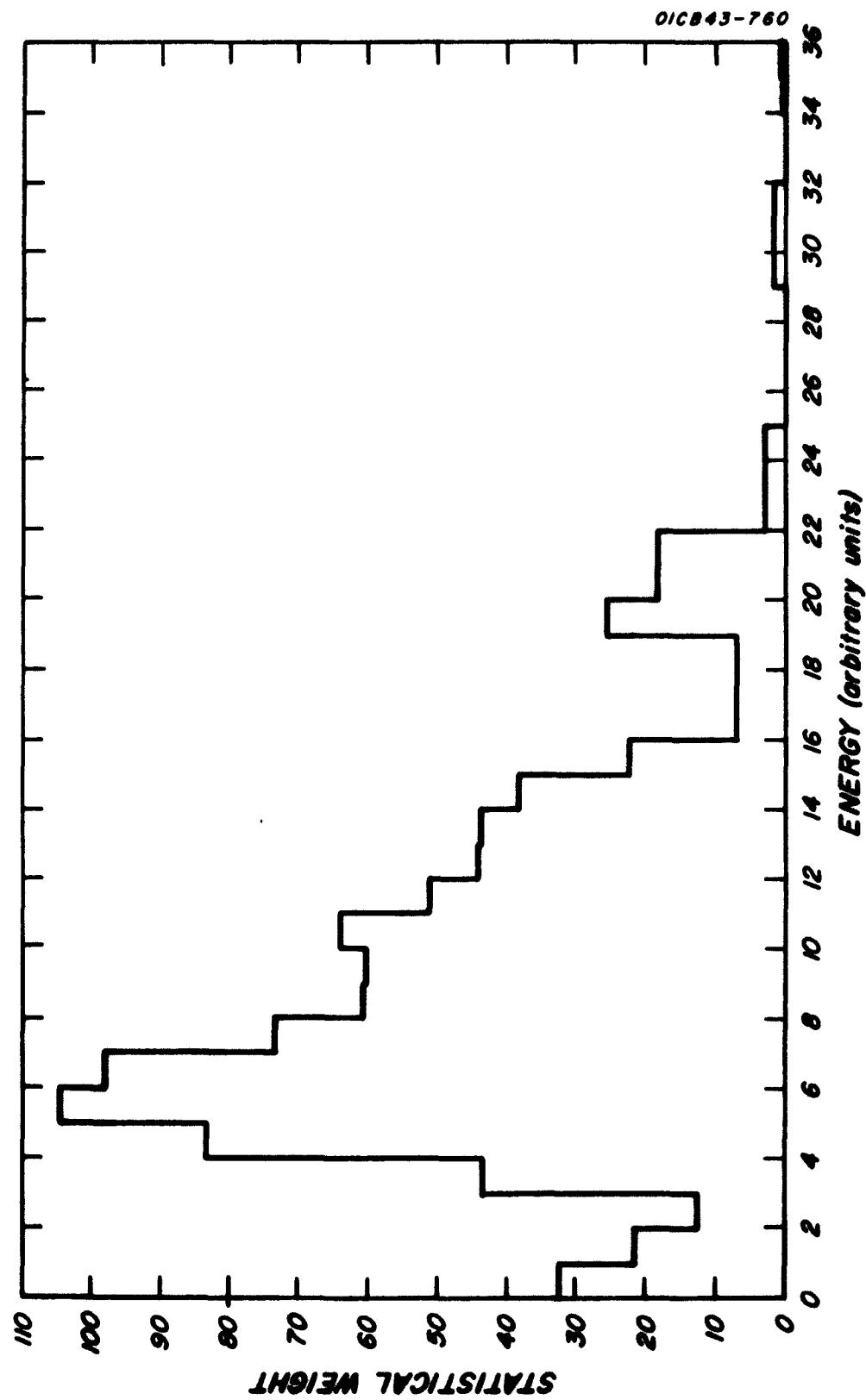


Figure F-6. Smoothed Distribution of Theoretical Energy Level in the Configuration f^4 .

distribution. In every case the main peak of the distribution lies significantly to the right of the lower cut-off.

Another defect of the exponential distribution consists in its not having the lower cut-off in the right place. The lower cut-off has in fact been arbitrarily placed σ_w units below the mean energy \bar{W} . This assignment is usually in error by a quantity not much smaller than σ_w itself. Thus the main features of the distribution are not as well represented by the exponential law as one would like.

We have sought to improve the statistical description in two ways. First, we have added a third parameter, which can in every case be calculated exactly with comparatively little labor. Secondly, we have chosen the distribution function in accordance with an objective principle -- the principle of maximum entropy inference -- which ensures that the probability distribution incorporates the maximum possible uncertainty consistent with having the correct mean, variance, and lower cut-off. These two improvements are discussed in detail in the following subsections.

F.5. The Lower Cut-off

The lower cut-off is simply the energy of the ground state of the configuration. Now, according to a well-known rule of Hund, the lowest spectroscopic term in a given configuration is the one with the highest value of S ; or, if two or more terms have the same value of S , the one of these with the highest value of L . One of the levels belonging to this

term, namely, the level with $M_S = S$ and $M_L = L$, is characterized not only by definite values of M_L , S , M_S , and the one-electron azimuthal quantum numbers l^i , but also by definite values of the one-electron magnetic quantum numbers m_l^i . Hence the corresponding wavefunction is a Slater determinant, and the corresponding energy can be obtained by a straightforward calculation. As an example we calculate the energy of the ground state of the configuration f^7 . (See Section F-9)

F.6. Maximum Entropy Inference

Consider the problem of determining the probability distribution $p(x)$ associated with a given random variable X . Suppose that the possible values of X are known to lie in the range (a, b) and that the first k moments of X are also known:

$$\mu_i = \int_a^b x^i p(x) dx \quad (i = 1, \dots, k) . \quad (F-8)$$

$p(x)$ must satisfy the further conditions

$$p(x) > 0, \quad \int_a^b p(x) dx = 1 . \quad (F-9)$$

According to the principle of maximum entropy inference (Jaynes ^(F-6)) the best choice for the function $p(x)$ is the one that maximizes the entropy

$$H = - \int_a^b p(x) \ln p(x) dx , \quad (F-10)$$

subject to the $k + 1$ auxiliary conditions expressed by the above integral equations. Using the method of Lagrange multipliers, one easily finds that $p(x)$ must have the form

$$p(x) = N \exp [a_1 x + a_2 x^2 + \dots + a_k x^k] . \quad (F-11)$$

The constants $a_1 \dots a_k$, N , can be found from the $k + 1$ integral conditions.

The entropy of a probability distribution is a measure of the uncertainty inherent in the distribution. Shannon (F-7) showed that no other function can consistently bear this interpretation. Thus the principle of maximum entropy inference may fairly be described as the correct method for choosing a probability distribution when partial information about the distribution exists. As Jaynes (F-6) has pointed out, it is a quantitative embodiment of Laplace's principle of insufficient reason.

F. 7. Application to the Distribution of Energy Levels in a Configuration

We now have three parameters at our disposal -- the mean energy \bar{W} , the standard deviation of the energy σ_w , and the energy of the ground state, which we denote by W_0 . Let

$$x = (W - W_0)/\epsilon , \quad (F-12)$$

where ϵ is an as yet unspecified unit of energy. The variable x is a dimensionless measure of the energy relative to the ground state.

Applying the principle of maximum entropy inference, we find that the probability distribution has the form

$$p = N \exp [-(x - b)^2] \quad (x > 0) . \quad (F-13)$$

The energy unit ϵ has been chosen so as to make the coefficient of x^2 in the exponential -1 . By integrating the last equation over the range of x we obtain a formula for the normalization constant N :

$$N = 2\pi^{-\frac{1}{2}} [1 + \operatorname{erf}(b)]^{-1} \quad (F-14)$$

where $\operatorname{erf}(x)$ is the error function

$$\operatorname{erf}(x) = 2\pi^{-\frac{1}{2}} \int_0^x e^{-y^2} dy . \quad (F-15)$$

Thus $p(x)$ depends on the single parameter b .

Let

$$\mu = (\bar{w} - w_0)/\epsilon , \quad \sigma = \sigma_w/\epsilon ; \quad (F-16ab)$$

μ and σ are the mean energy and the standard deviation in dimensionless units.

The integral conditions which ensure that the probability distribution has the required mean and variance yield two independent relations from which b and ϵ can be evaluated in terms of μ and σ . The following form of these relations is convenient for calculation:

$$\mu = b + \frac{1}{2}p(0) , \quad (F-17)$$

$$(\sigma/\mu)^2 = [1 - \mu p(0)]/2\mu^2 . \quad (F-18)$$

By substituting the first equation into the second, we obtain a transcendental equation for b in terms of the ratio (σ/μ) . The numerical solution of this equation for a range of values of σ/μ can be obtained easily. Table F-1 gives σ/μ for various values of b , and the same is plotted in Figure F-7. Having obtained the value of b from this table, one can evaluate the energy unit ϵ from equations (F-17) and (F-16a).

The agreement between the predicted and observed distributions seems to be satisfactory. If future studies should disclose a systematic discrepancy between the predicted and observed distribution, then the very existence of such discrepancies would represent fresh information about the probability distribution and could be incorporated into the conditions of the problem. Moreover, it is likely that any such systematic discrepancy would have an assignable physical cause. Thus the principle of maximum entropy inference appears to be a powerful method for isolating those properties of complex spectra that are susceptible to interpretation in reasonably simple terms.

F.8. Statistical Description of the Combination Spectra

Consider a transition array, defined as the aggregate of lines resulting from all possible transitions connecting two

TABLE F-1

$\frac{Q}{\mu}$ and b

b	$\frac{Q}{\mu}$
0.0	.75122
0.1	.70515
0.25	.63495
0.5	.59937
0.75	.57272
1.0	.53512
1.25	.48832
1.5	.43851
1.75	.39107
2.0	.34742
2.5	.28235
3.0	.23567
3.5	.20203
4.0	.17677

subject to the $k + 1$ auxiliary conditions expressed by the above integral equations. Using the method of Lagrange multipliers, one easily finds that $p(x)$ must have the form

$$p(x) = N \exp [a_1 x + a_2 x^2 + \dots + a_k x^k] . \quad (F-11)$$

The constants $a_1 \dots a_k$, N , can be found from the $k + 1$ integral conditions.

The entropy of a probability distribution is a measure of the uncertainty inherent in the distribution. Shannon (F-7) showed that no other function can consistently bear this interpretation. Thus the principle of maximum entropy inference may fairly be described as the correct method for choosing a probability distribution when partial information about the distribution exists. As Jaynes (F-6) has pointed out, it is a quantitative embodiment of Laplace's principle of insufficient reason.

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$$x = (W - W_0)/\epsilon , \quad (F-12)$$

where ϵ is an as yet unspecified unit of energy. The variable x is a dimensionless measure of the energy relative to the ground state.

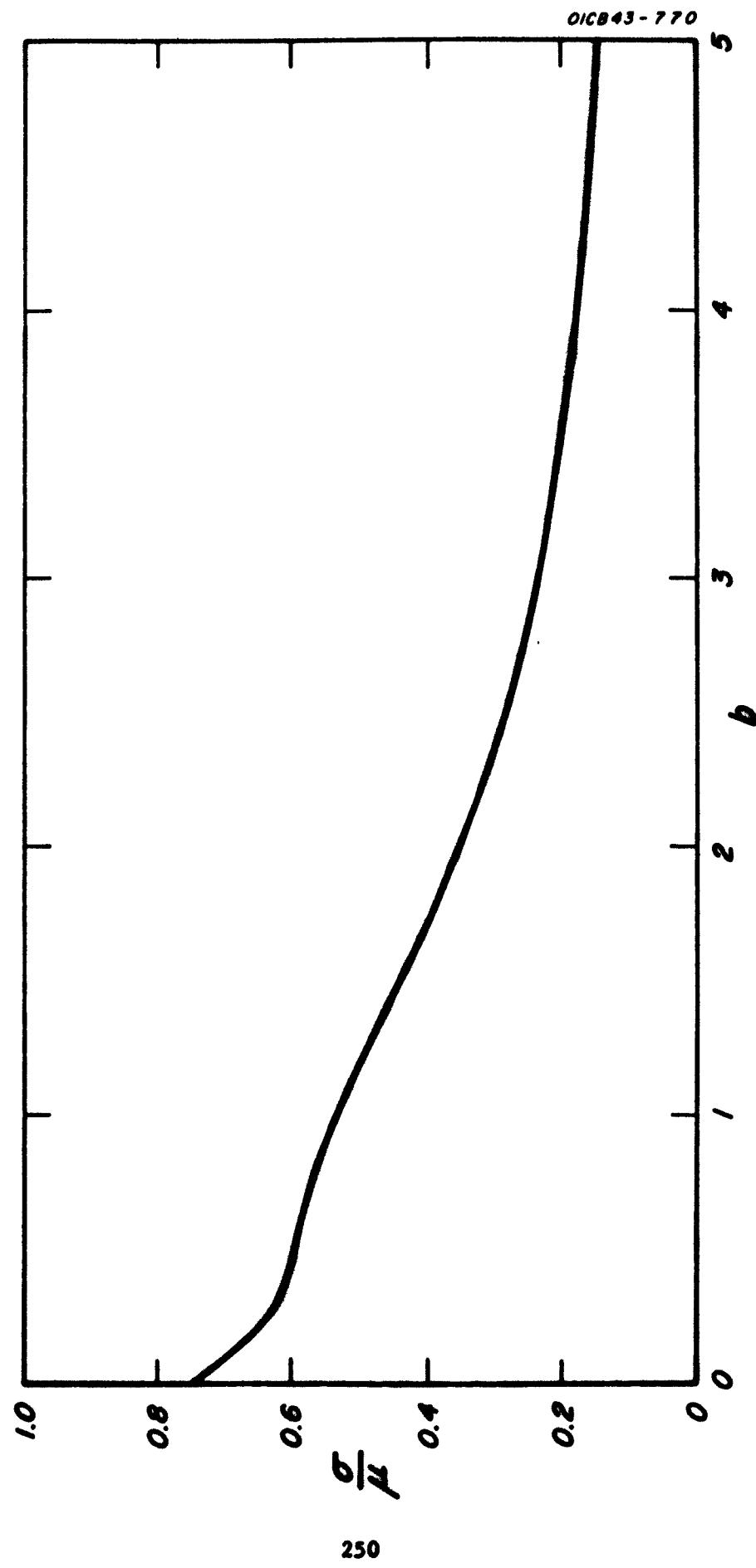


Figure F-7. Solution to Equations F-17 and F-18.

given configurations. What can we say about the probability distribution of line frequencies in such an array, given the probability distributions for the energy levels of the two configurations?

Let W_{ai} denote the energy of the i th level in the configuration a. The frequency corresponding to a transition $a_i \rightarrow b_j$ is given by Bohr's frequency condition,

$$h\nu(ai, bj) = W_{ai} - W_{bj} . \quad (F-19)$$

We assume for the sake of definiteness that configuration a lies above configuration b, so that the frequencies defined by this equation are always positive.

If departures from LS coupling are not too great, the combination spectrum [the spectrum of frequencies $\nu(ai, bj)$] will have a clumpy structure. Transitions between levels belonging to the same pair of spectroscopic terms give rise to multiplets, and in LS coupling the separation between multiplets is large compared with the separation between lines in a multiplet.

The distribution of lines in a multiplet and the distribution of multiplets in a transition array present distinct problems. In a first approximation we may assume that the two distributions are stochastically independent -- that is,

that the form of the probability distribution for lines in a multiplet does not depend on the position of the multiplet in its transition array. Similar remarks apply to the case of pure jj coupling.

On the other hand, if the coupling scheme is not close to either LS or jj coupling, neither the individual energy spectra nor the combination spectrum will exhibit any marked fine structure. In this respect the case of intermediate coupling is easier to deal with than either extreme LS coupling or extreme jj coupling.

There is a second important respect in which the stochastic description of the combination spectrum is simpler for intermediate coupling than for LS coupling. In LS coupling, transitions connecting levels belonging to terms of different multiplicity (different S) are strictly forbidden. This well-known selection rule substantially reduces the number of lines in a transition array that occur with nonvanishing intensity. Moreover, it forces one to deal separately with the various classes of transitions corresponding to the various possible values of S. In jj coupling transitions connecting terms differing by more than one quantum number j are forbidden. In intermediate coupling, on the other hand, intersystem transitions are not only allowed, but often have high probability. Since intermediate coupling prevails in heavy atoms, we may reasonably assume that the choice of an initial level and the choice of a final level are stochastically independent events. The remainder of this discussion proceeds from this assumption.

If we regard the quantities v , W_a , W_b as random variables [whose possible values are the numbers $v(a_i, b_j)$, W_{a_i} , W_{b_j} , respectively], then the assumption just stated means that the random variables W_a and W_b are stochastically independent, so that the random variable v is the difference between two stochastically independent random variables. This fact enables us to write down the probability distribution of v in terms of the probability distributions of W_a and W_b : According to a well-known theorem in probability theory, the first distribution is just the convolution of the probability distributions of W_a and W_b . Let $p_a(x)$ denote the probability distribution of W_a and \bar{p}_b denote the probability distribution of $-W_b$. Then the probability distribution p_{ab} of

$$W_{ab} = W_a - W_b \quad (F-20)$$

is given by

$$p_{ab}(y) = \int_{-\infty}^{\infty} p_a(x) \bar{p}_b(y - x) dx. \quad (F-21)$$

From this equation, or, more directly, from the definition of stochastic independence, one can show that the expectation and the variance of W_{ab} are given by

$$\bar{W}_{ab} = \bar{W}_a - \bar{W}_b, \quad (F-22)$$

$$\text{Var } W_{ab} = \text{Var } W_a + \text{Var } W_b. \quad (F-23)$$

As an illustration of these rules we consider the example of two normal distributions. By an appropriate choice of zero-points we can always ensure that $\bar{W}_a = \bar{W}_b = \bar{W}_{ab} = 0$, so that we

may put

$$p_a(x) = (2\pi\sigma_a^2)^{-\frac{1}{2}} \exp [-x^2/2\sigma_a^2], \quad (F-24)$$

$$p_b(x) = (2\pi\sigma_b^2)^{-\frac{1}{2}} \exp [-x^2/2\sigma_b^2]. \quad (F-25)$$

Since the normal probability distribution is symmetric, the probability distribution \bar{p}_b of $-W_b$ coincides with p_b in the present example; but this is not true in general. A short calculation, in which one performs the integration by completing the square in the exponent, gives

$$p_{ab}(x) = (2\pi\sigma_{ab}^2)^{-\frac{1}{2}} \exp [-x^2/2\sigma_{ab}^2], \quad (F-26)$$

$$\sigma_{ab}^2 = \sigma_a^2 + \sigma_b^2; \quad (F-27)$$

the probability distribution of the difference W_{ab} is also normal and its variance is the sum of the variances of W_a and W_b . This is the well-known "reproductive property" of the normal distribution.

We assume that the probability distributions p_a , p_b have the form derived earlier in the present report. It is convenient to introduce the function

$$\epsilon(x) = \begin{cases} 1 & (x > 0) \\ 0 & (x < 0) \end{cases} \quad (F-28)$$

With the help of this function we can write the probability distribution for W_a in the form

$$p_a(x) = \phi(x; \sigma_a, \beta_a) \epsilon(x), \quad (F-29)$$

where

$$\varphi(x; \sigma_a, \beta_a) = N_a \exp [-(x - \beta_a)^2 / 2\sigma_a^2] . \quad (F-30)$$

The definition of p_b is exactly analogous. Note that

$$\bar{p}_a(x) = p_a(-x) \quad (F-31)$$

We therefore obtain for the probability distribution of w_{ab}

$$p_{ab}(y) = \int_{-\infty}^{\infty} \varphi(x; \sigma_a, \beta_a) \varphi(x - y; \sigma_b, \beta_b) \epsilon(x) \epsilon(x - y) dx . \quad (F-32)$$

From the definition of the function $\epsilon(x)$ it follows at once that

$$\begin{aligned} \epsilon(x - y) &= (y > 0) \\ \epsilon(x) \epsilon(x - y) &= . \\ \epsilon(x) &= (y < 0) \end{aligned} \quad (F-33)$$

Hence

$$p_{ab}(y) = \int_0^{\infty} \varphi(x; \sigma_a, \beta_a) \varphi(x - y; \sigma_b, \beta_b) dx \quad (y < 0) ; \quad (F-34a)$$

$$\begin{aligned} p_{ab}(y) &= \int_y^{\infty} \varphi(x; \sigma_a, \beta_a) \varphi(x - y; \sigma_b, \beta_b) dx \\ &= \int_0^{\infty} \varphi(y + z; \sigma_a, \beta_a) \varphi(z; \sigma_b, \beta_b) dz \quad (y > 0) . \end{aligned} \quad (F-34b)$$

The integrations are straightforward (see the Mathematical Note at the end of this appendix). The final result is:

$$p_{ab}(y) = P_{ab}(y) \left[1 - \operatorname{erf} \left(\frac{\beta_a \beta_b^2 + \beta_b \sigma_a^2 + y \sigma_a^2}{\sigma_a \sigma_b \sqrt{2(\sigma_a^2 + \sigma_b^2)}} \right) \right] \quad (y < 0) \quad (F-35a)$$

$$= P_{ab}(y) \left[1 - \operatorname{erf} \left(\frac{\beta_a \beta_b^2 + \beta_b \sigma_a^2 - y \sigma_b^2}{\sigma_a \sigma_b \sqrt{2(\sigma_a^2 + \sigma_b^2)}} \right) \right] \quad (y > 0) \quad (F-35b)$$

$$\text{where } P_{ab}(y) = \frac{1}{2} N_a N_b \left[\frac{2\pi}{\sigma_a^2 + \sigma_b^2} \right]^{1/2} \sigma_a \sigma_b \exp \left[- \frac{(\beta_a - \beta_b - y)^2}{2(\sigma_a^2 + \sigma_b^2)} \right]$$

and $\operatorname{erf}(x)$ has been defined in equation (F-15)

F.9. Ground State Energy for a Configuration of Equivalent Electrons

We consider a configuration of equivalent electrons ℓ^q . The energy of the completely filled shells is common to all the terms of the configuration, ℓ^q . It can be calculated, if desired, but is of no consequence for our purpose. Furthermore, the average energy of such a configuration can be calculated in a straightforward manner (Slater^(F-2)).

$$W_{av}(\ell^q) = \frac{q(q-1)}{2} \quad W_{av}(\ell^2) \quad (F-36)$$

$$\text{and } W_{av}(\ell^2) = \sum_k^{2\ell} f^k(\ell, \ell) F^k(n\ell, n\ell) \quad (F-37)$$

where the coefficients f^k for configurations of p, d, f and g electrons are given in Table B-1 and F^k are the Slater F integrals defined in Equations (B-26) and (B-27).

We shall describe below a method of calculating the energy of the ground term.

It is well known that a subshell ℓ can contain at most $2(2\ell + 1)$ electrons and is therefore exactly half filled when $q = 2\ell + 1$. It is also well known that the term energies (with respect to the average energy) of a configuration with n electrons are the same as those of a configuration with $[2(2\ell + 1) - q]$ electrons. It is, therefore, necessary only to consider configurations which are half or less than half filled, i.e. $q \leq 2\ell + 1$.

The ground term of any configuration has the largest value of S for that configuration. If several terms have the same largest value of S , say S_{\max} , it is the one with the largest value of L , say L_{\max} , among them. Each term is highly degenerate, but one of the $SL M_S M_L$ states belonging to the term (S_{\max}, L_{\max}) is such that

$$M_S = S_{\max}$$

and $M_L = L_{\max}$.

The zero-order state, which belongs uniquely to the above set of values of the quantum numbers can be found easily. $M_S = S_{\max}$ arises when all spins are parallel and in this case m_s of all n electrons is $+\frac{1}{2}$ ($\text{or } -\frac{1}{2}$). Therefore,

$$M_S = S_{\max} = \frac{1}{2} q \quad (\text{P-38})$$

and the multiplicity of the ground term is $(2 S_{\max} + 1)$ or $(q + 1)$.

The largest value of M_L consistent with the above requirement on the m_s and M_S is obtained by a simple application of the exclusion principle.

The m_L values of the q equivalent electrons must be

$$m_L = \ell, \ell - 1, \dots, (\ell - q + 1) \quad (F-39)$$

For this case

$$M_L = L_{\max} = \frac{q}{2} (2\ell - q + 1) \quad (F-40)$$

The corresponding zero order state is designated in the usual way by

$$(\ell)^+ (\ell-1)^+ \dots (\ell - q + 1)^+$$

where the quantity in parenthesis is the value of m_L of individual electrons and the + sign indicates that $m_s = +1/2$. The ground terms of a few configuration of type ℓ^n are given in Table F-2. For a shell which is exactly half filled ($q = 2\ell + 1$), it is readily seen from Equation (F-5) that $L_{\max} = 0$ and the term is $(2\ell + 2)_S$.

TABLE F-2

Ground Terms for Configurations of Equivalent Electrons

Configuration	Multiplicity [= $q + 1$]	L [= $\frac{q}{2} (2\ell - q + 1)$]	Ground Term
p^2	3	1	3p
d^3	4	3	4F
f^7	8	0	8S
g^5	6	10	6N

The energy of the ground term in the absence of external fields is the same as that of any one of the zero order states of this term, say of the zero order state mentioned above. This energy can be found by standard methods (Condon and Shortley^(F-3)), and is given by,

$$W = \sum_{\alpha > \beta} \sum_k \left[a^k (\ell m_{\ell}^{\alpha}, \ell m_{\ell}^{\beta}) - b^k (\ell m_{\ell}^{\alpha}, \ell m_{\ell}^{\beta}) \right] F^k (n\ell, n\ell) \quad (F-41)$$

where the first summation is over all two electrons combinations and the second summation is over k which takes on all even values from zero to 2ℓ . The coefficients a^k and b^k are defined by Equations 8⁶ (14) and 8⁶ (6) of Condon and Shortley^(F-3), and are tabulated by them in Tables 1⁶ and 2⁶ for s, p, d and f electrons.

As an example we calculate below the energy of the ground term of configuration f^7 . The zero order state of lowest energy is

$$3^+ 2^+ 1^+ 0^+ -1^+ -2^+ -3^+$$

and uniquely belongs to the 8S term. Table F-3 gives the appropriate a^k and b^k for f electrons. From the sums of these quantities, given in the last row of this table, it readily follows that the energy of the ground term, 8S , of the configuration f^7 is

TABLE F-3

 $a^k (\ell m_\ell^\alpha, m_\ell^\beta)$ and $b^k (\ell m_\ell^\alpha, \ell m_\ell^\beta)$ for f-electrons
Note: $a^0 = 1$ for all cases $b^0 = 0$ if $m_\ell^\alpha \neq m_\ell^\beta$

Electrons		a^2	a^4	a^6	b^2	b^4	b^6	
α	β	$\times 225$	$\times 1089$	$\times 7361.64$	$\times 225$	$\times 1089$	$\times 7361.64$	
3 ⁺	2 ⁺	0	-21	-6	25	30	7	
	1 ⁺	-15	3	15	10	54	28	
	0 ⁺	-20	18	-20	0	63	84	
	-1 ⁺	-15	3	15	0	42	210	
	-2 ⁺	0	-21	-6	0	0	462	
	-3 ⁺	25	9	1	0	0	924	
	2 ⁺	1 ⁺	0	-7	-90	15	32	105
2 ⁺	0 ⁺	0	-42	120	20	3	224	
	-1 ⁺	0	-7	-90	0	14	378	
	-2 ⁺	0	49	36	0	70	504	
	-3 ⁺	0	-21	-6	0	0	462	
	1 ⁺	0 ⁺	12	6	-300	2	15	350
	-1 ⁺	9	1	225	24	40	420	
	-2 ⁺	0	-7	-90	0	14	378	
1 ⁺	-3 ⁺	-15	3	15	0	42	210	
	0 ⁺	-1 ⁺	12	6	-300	2	15	350
	-2 ⁺	0	-42	120	20	3	224	
	-3 ⁺	-20	18	-20	0	63	84	
	-1 ⁺	-2 ⁺	0	-7	-90	15	32	105
	-3 ⁺	-15	3	15	10	54	28	
	-2 ⁺	-3 ⁺	0	-21	-6	25	30	7
\sum		-42	-77	-462	168	616	5544	

$$W(f^7 \ ^8S) = 21F^0 - \frac{210}{225} F^2 - \frac{693}{1089} F^4 - \frac{6006}{7361.64} F^6 \quad (F-42).$$

F.10. Mathematical Note

From Equations (F-30) and F-34a) we obtain, for $y < 0$,

$$p_{ab}(y) = N_a N_b \int_0^\infty \exp \left[-\frac{(x - \beta_a)^2}{2 \sigma_a^2} - \frac{(x - y - \beta_b)^2}{2 \sigma_b^2} \right] dx \quad (F-43a)$$

$$= N_a N_b \int_0^\infty \exp \left[-\left(mx^2 + 2qx + r \right) \right] dx \quad (F-43b)$$

where

$$m = \frac{\sigma_a^2 + \sigma_b^2}{2 \sigma_a^2 + \sigma_b^2} \quad (F-44a)$$

$$q = \frac{-\beta_a \sigma_b^2 + (y + \beta_b) \sigma_a^2}{2 \sigma_a^2 \sigma_b^2} \quad (F-44b)$$

$$r = \frac{\beta_a^2 \sigma_b^2 + (y + \beta_b)^2 \sigma_a^2}{2 \sigma_a^2 \sigma_b^2} \quad (F-44c)$$

The integral on the right hand side of Equation (F-43b) can be evaluated by means of formula (6b), Table 314, page 65 of the compilation of definite integrals by Gröbner and Hofreiter^(F-10). Applying this formula we obtain Equation (F-35a).

For $y > 0$, we combine Equations (F-30) and (F-34b) and get

$$p_{ab}(y) = N_a N_b \int_0^\infty \exp \left[-\frac{(z - (-y + \beta_a))^2}{2 \sigma_a^2} - \frac{(2 - \beta_b)^2}{2 \sigma_b^2} \right] dx \quad (F-45)$$

which is the same as Equation (F-42a) if we interchange the subscripts a and b and replace y by (-y). Performing the integration as before we obtain Equation (F-35b).

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APPENDIX G
H. E. Stubbs and G. A. Victor

THE EFFECT OF LINE WIDTH, STRENGTH, AND SHAPE
ON RADIATIVE TRANSFER IN AN EXPANDING GAS

G.1 Introduction

The details of line width, shape, and strength have a very important role in the calculation of radiative transfer phenomena in non-expanding gas clouds. This dependence on details of line shape introduces very serious complications in most astrophysical applications^(G-1,2), since reliable information on line shapes is available only for simple gases as hydrogen and helium^(G-3). The object of this appendix is to investigate a simple model of a rapidly expanding gas which results in expressions for line absorption which are largely independent of detail line shape. The origin of the simplification in this model is found in the fact that the Doppler shift due to the velocity of expansion becomes the dominant factor, and that the details of line shape due to collision and thermal Doppler broadening become unimportant.

This appendix will be divided into three sections. Part G.2 will be devoted to some simple estimations of line widths due to the thermal Doppler broadening, and to compare it with the Doppler shift due to the expansion velocity. Part G.3 will show that resonance absorption is independent of line shape. Part G.4 will present a simple calculation for an expanding hydrogen gas for the transmission of the 82, 260 cm^{-1} line.

G.2 Doppler Shift Due to Velocity of Expansion

We shall construct the following idealized model for our expanding cloud:

The number density of hydrogen atoms is given by:

$$\begin{aligned}\rho(r,t) &= 1.5 \times 10^3 / t^3 \text{ particles/cm}^3 \quad r < R_o(t) \\ \rho(r,t) &= 0 \quad r > R_o(t) \\ R_o(t) &= V_o t \\ V_o &= 1 \times 10^{-2} \text{ cm/sec.}\end{aligned}\tag{G-1}$$

t is the time in seconds

c is the speed of light = 3×10^{10} cm/sec.

the relative velocity between two particles is along their line of centers and is given by:

$$v_{\text{rel}} = \frac{r_{12}}{t} \tag{G-2}$$

Where r_{12} is the particles separation:

The relativistic Doppler formula is:

$$\lambda = \lambda_o \beta \cos \theta \tag{G-3}$$

Since the velocity is along the line of centers we can set $\cos \theta = 1$.

Since $v_{\text{rel}} \ll c$ we have the relation $\beta_{\text{MAX}} = .02$. therefore:

$$\lambda_{\text{MAX}} = .02 \lambda_o \tag{G-4}$$

The formula for the thermal Doppler width is

$$3\lambda_T = \lambda \left[\frac{2kT \log 2}{Mc^2} \right]^{1/2} \quad (G-5)$$

for Hydrogen we can construct the following table:

$3/2 kT$	$\delta\lambda_T$	$3\lambda_T / \lambda_{MAX}$
100 ev	$3.2 \times 10^{-4} \lambda_0$	1.6×10^{-2}
10 ev	$10^{-4} \lambda_0$	5.0×10^{-3}
1 ev	$3.2 \times 10^{-5} \lambda_0$	1.6×10^{-3}
.1 ev	$10^{-5} \lambda_0$	5×10^{-4}

From Table G-1 we see that the Doppler width due to thermal motion is always much smaller than the maximum Doppler shift due to the velocity of expansion. The results of the rest of this appendix depend on this fact.

G.3 Independence of Resonance Absorption on Line Shape

Let a photon of frequency ω be emitted at $r = 0$. Let the probability of emission of a photon of energy between $\hbar\omega$ and $\hbar(\omega + dw)$ per unit time per particle be given by $P(\omega)$. The probability that a given atom will absorb a photon of energy $\hbar\omega$ is given by,

$$p(\omega) = k P(\omega) \quad (G-6)$$

from the principle of detail balance.

The probability that a photon of frequency ω will transverse a distance r before being absorbed is given by:

$$I(\omega, r) = e^{- \int_0^r A(\xi, \omega) d\xi} \quad (G-7)$$

with

$$A(\xi, \omega) = \rho(\xi) p(\omega'[\xi, \omega_0]) \quad (G-8)$$

where $\rho(\xi)$ is the density of particles which can absorb this resonance radiation. $I(\omega, r)$ can therefore be written as:

$$I(\omega, r) = e^{- \int_0^r \rho(\xi) p(\omega[1 - \frac{\xi}{ct_0}]) d\xi} \quad (G-9)$$

where we have used the Doppler formula:

$$\Delta\omega = \frac{\omega\xi}{ct} \quad (G-10)$$

and evaluated this at a particular time t_0 .

We integrate this over all frequencies, weighted with $P(\omega)$ to get the probability that any photon will go a distance r .

$$T(r) = \int_{-\infty}^{+\infty} d\omega P(\omega) e^{- \int_0^r d\xi \rho(\xi) p(\omega[1 - \frac{\xi}{ct_0}])} \quad (G-11)$$

which will be re-written as

$$T(r) = \int_{-\infty}^{+\infty} d\omega P(\omega) e^{-k \int_0^r d\xi \rho(\xi) P(\omega[1 - \frac{\xi}{ct_0}])} \quad (G-12)$$

If $\rho(\xi)$ is a constant out to a distance r , which is consistent with our cloud model, we have:

$$T(r) = \int_{-\infty}^{+\infty} d\omega P(\omega) e^{+ K' \int_{\omega}^{\omega + \Delta\omega(r)} P(\xi) d\xi} \quad (G-13)$$

where: $K' = kp$ $\Delta\omega(r) = \frac{\omega r}{ct_0}$

Finally

$$T(r) = \int_{-\infty}^{+\infty} P(\omega) d\omega e^{+ \int_{\omega}^{\omega(1 - \frac{r}{dt})} K' P(\omega') d\omega'} \quad (G-14)$$

Using the result of part G.2 we can calculate this for $r = \infty$

$$T(\infty) = \int_{-\infty}^{+\infty} P(\omega) d\omega e^{K' \int_{\omega}^{-\infty} P(\omega') d\omega'} \quad (G-15)$$

if we let $\eta = \int_{-\infty}^{\omega} P(\omega') d\omega'$

then $d\eta = P(\omega) d\omega$

so:

$$T(\infty) = \int_0^1 d\eta e^{-K'\eta} = \left[\frac{1}{K'} (1 - e^{-K'}) \right] \quad (G-16)$$

From Equation (G-16) we see that for an infinite cloud

resonance absorption is independent of line shape. For a finite cloud, it is only the photons that are emitted near the edge that will show resonance absorption that is dependent on the form of $P(\omega)$. The ratio of the thickness of this edge to the cloud radius is essentially $\delta\lambda_T/\Delta\lambda_{MAX}$. We therefore conclude that resonance absorption is controlled primarily by line strength, for this simple model of an expanding cloud. The object of this appendix is to investigate a simple model of a rapidly expanding gas which results in expressions for line absorption which are largely independent of detail line shape.

Arguments similar to those given above for resonance absorption can be given for line absorption due to two close, but non-overlapping lines. It is easy to see that an absorption line centered at λ_0 can only absorb radiation from lines centered at λ_1 such that:

$$\lambda_0 - \lambda_1 < \Delta\lambda_{MAX} \approx .04\lambda_0 \quad (G-17)$$

It is again obvious that this absorption is independent of line shape except for lines where the equality holds in Equation (G-17). The effect of a finite cloud on the absorption of non-overlapping line radiation does little but introduce some simple geometrical factors.

G.4 Transmission of Hydrogen $82,260 \text{ cm}^{-1}$ Line

The line of interest is the $82,260 \text{ cm}^{-1}$ line which is emitted by a transition from the first excited state to the ground state. We will assume that the gas has a temperature history as shown in Figure G-1. In addition, we assume that the gas is at thermal equilibrium at all times.

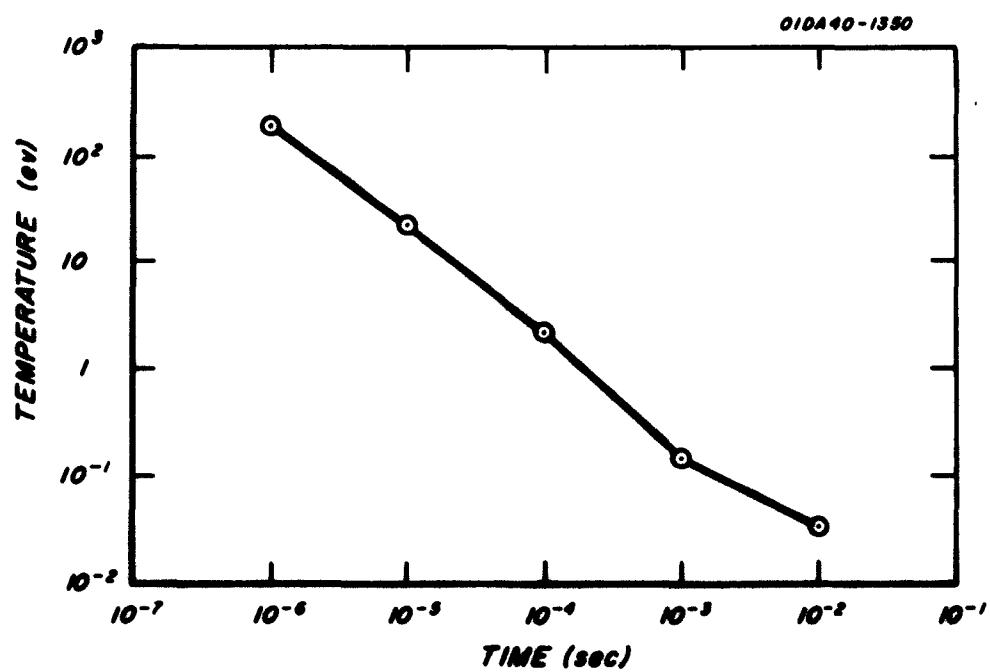


Figure G-1. Temperature During Expansion.

At equilibrium, the population of states is given by the Saha equation

$$N_n = N_p N_e n^2 h^3 [2\pi m k T]^{-3/2} \exp \frac{I_r - I_{r,n}}{k T} \quad (G-18)$$

N_p = number density of protons

N_e = number density of electrons

I_r = ionization potential (r degree)

n = principle quantum number

N_n = number density of atoms in state n

The number density of particles which can absorb the $82,260 \text{ cm}^{-1}$ line is given by

$$\rho(t, T) = \rho_0(t) f(t, T) \quad (G-19)$$

where $f(t, T) = \frac{N_1(T)}{\rho_0(t)}$

Estimations of $f(t, T)$ from Equation (G-18) lead to the results shown in the following table.

Time	ρ_0 [particles/cm ³]	R [cm]	K_t	f_t	T_∞
10^{-6}	1.5×10^{21}	2×10^2	$7 \times 10^7 f$	5.7×10^4	2.5×10^{-5}
10^{-5}	1.5×10^{18}	2×10^3	$7 \times 10^5 f$	1.08×10^{-5}	1.3×10^{-1}
10^{-4}	1.5×10^{15}	2×10^4	$7 \times 10^3 f$.26	1.4×10^{-4}
10^{-3}	1.5×10^{12}	2×10^5	$7 \times 10^1 f$	1	1.4×10^{-2}
10^{-2}	1.5×10^9	2×10^6	$7 \times 10^{-1} f$	1	

From Equation (G-16) we have:

$$T_t(\infty) = \frac{1}{K'_t} \left(1 - e^{-K'_t t} \right) \quad (G-20)$$

where the subscript indicates time dependence. K'_t is given by the following expression:

$$K'_t = \frac{\rho(t, T) R(t) A}{8\pi \nu^3 V_0} = \frac{\rho(t, T) A t}{8\pi \nu^3} \quad (G-21)$$

A is the Einstein coefficient $\sim 5 \times 10^8 \text{ sec}^{-1}$. The results for K'_t at various times is shown in Table G-2. Figures G-2 and G-3 show the variation of $T(\infty)$ with time for this simple model.

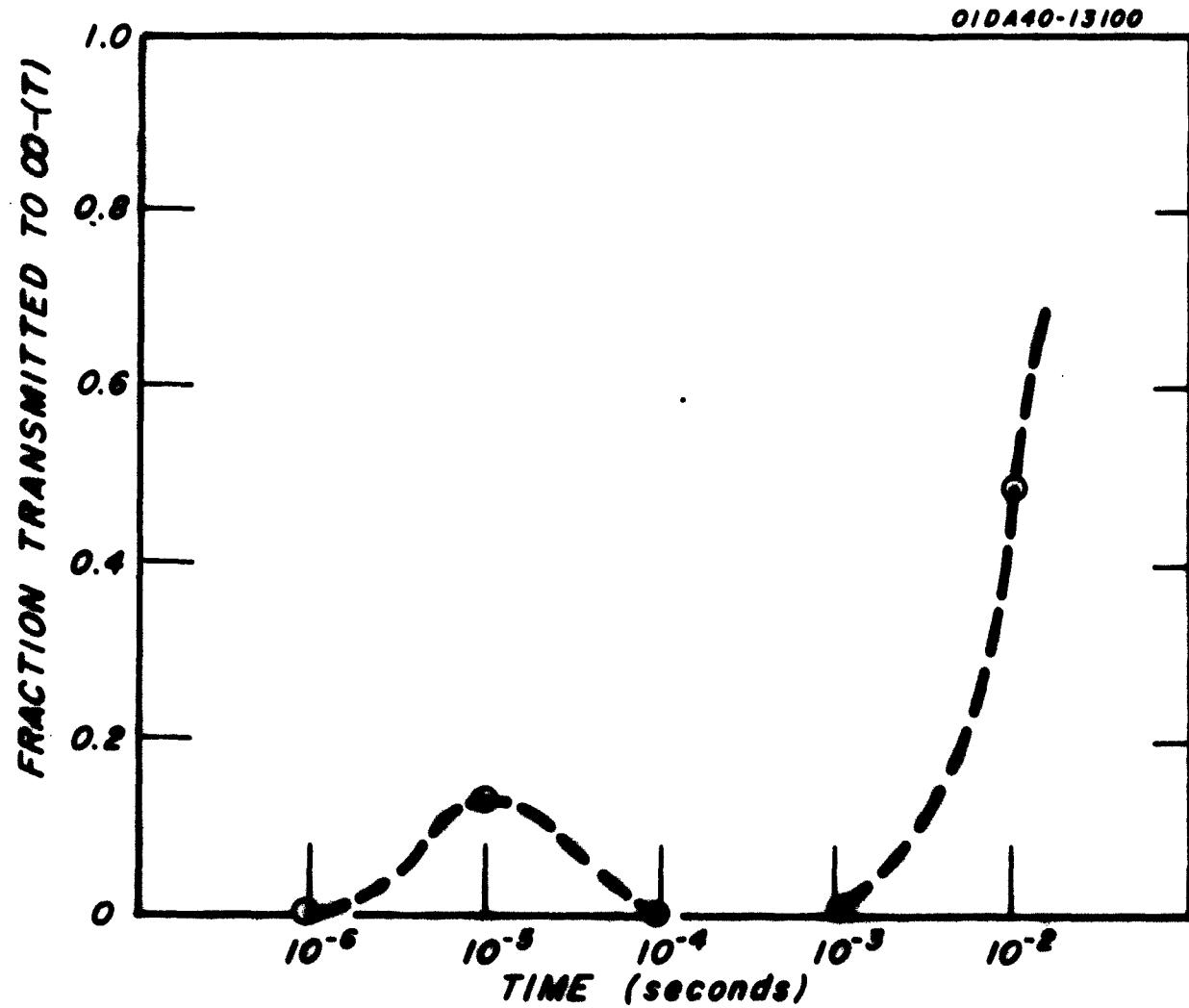


Figure G-2. Transmission in Expanding Medium.

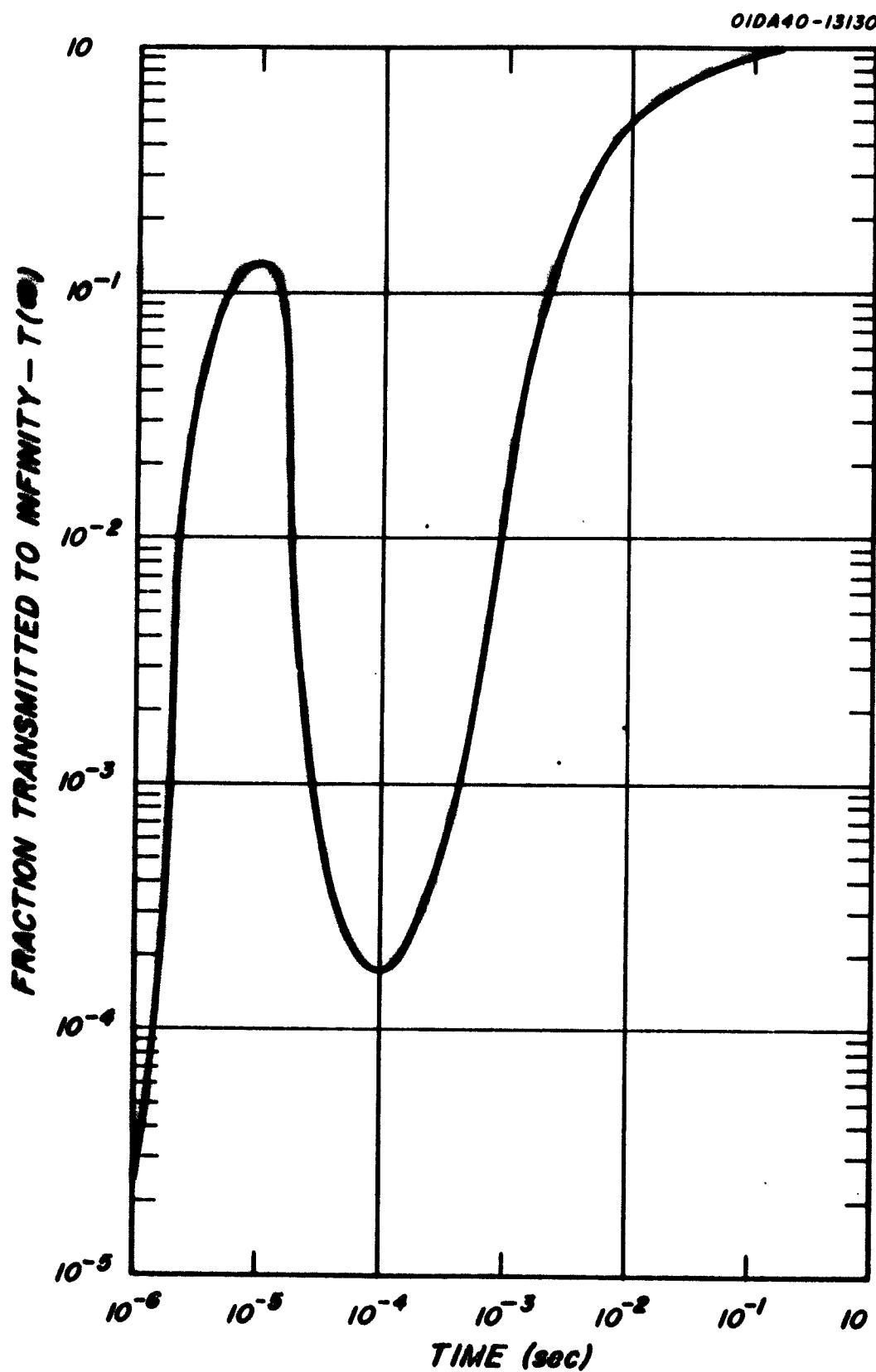


Figure G-3. Fraction of Photons escaping

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